



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2026 – 12:13 PM JST

PDB ID : 9VIA / pdb_00009via
Title : Crystal structure of fused glycerol dehydratase M158W variant
Authors : Park, R.Y.; Seo, M.D.
Deposited on : 2025-06-18
Resolution : 3.68 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

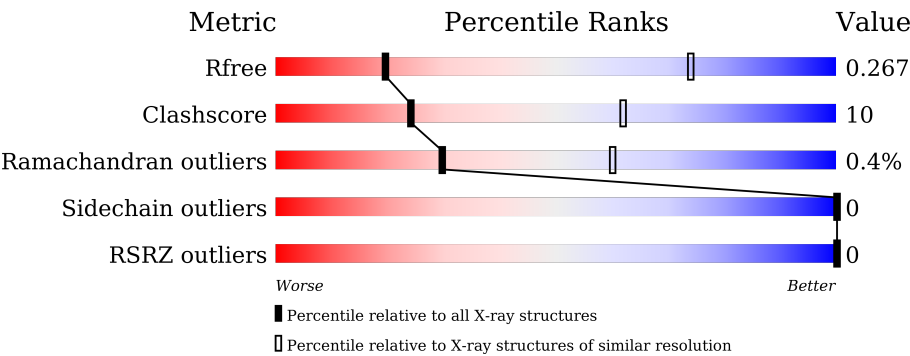
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1263 (3.80-3.56)
Clashscore	190562	1305 (3.80-3.56)
Ramachandran outliers	187476	1259 (3.80-3.56)
Sidechain outliers	187428	1256 (3.80-3.56)
RSRZ outliers	180081	1262 (3.80-3.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	754	<div><div></div><div>74%24%.</div></div>
1	C	754	<div><div></div><div>75%23%.</div></div>
1	F	754	<div><div></div><div>72%25%.</div></div>
1	G	754	<div><div></div><div>77%22%.</div></div>
2	D	141	<div><div></div><div>71%26%.</div></div>
2	E	141	<div><div></div><div>88%11%.</div></div>

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Mol	Chain	Length	Quality of chain
2	H	141	 82% 18% .
2	I	141	 83% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27597 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycerol dehydrase alpha subunit,Glycerol dehydrase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	744	Total	C	N	O	S	0	0	0
			5694	3558	998	1106	32			
1	C	746	Total	C	N	O	S	0	0	0
			5721	3573	1005	1110	33			
1	F	736	Total	C	N	O	S	0	0	0
			5629	3516	989	1092	32			
1	G	747	Total	C	N	O	S	0	0	0
			5722	3574	1004	1111	33			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	556	GLN	-	linker	UNP Q59476
B	557	GLY	-	linker	UNP Q59476
B	558	GLY	-	linker	UNP Q59476
B	559	ILE	-	linker	UNP Q59476
B	560	PRO	-	linker	UNP Q59476
B	561	VAL	-	linker	UNP Q59476
B	718	TRP	MET	engineered mutation	UNP O08505
C	556	GLN	-	linker	UNP Q59476
C	557	GLY	-	linker	UNP Q59476
C	558	GLY	-	linker	UNP Q59476
C	559	ILE	-	linker	UNP Q59476
C	560	PRO	-	linker	UNP Q59476
C	561	VAL	-	linker	UNP Q59476
C	718	TRP	MET	engineered mutation	UNP O08505
F	556	GLN	-	linker	UNP Q59476
F	557	GLY	-	linker	UNP Q59476
F	558	GLY	-	linker	UNP Q59476
F	559	ILE	-	linker	UNP Q59476
F	560	PRO	-	linker	UNP Q59476
F	561	VAL	-	linker	UNP Q59476

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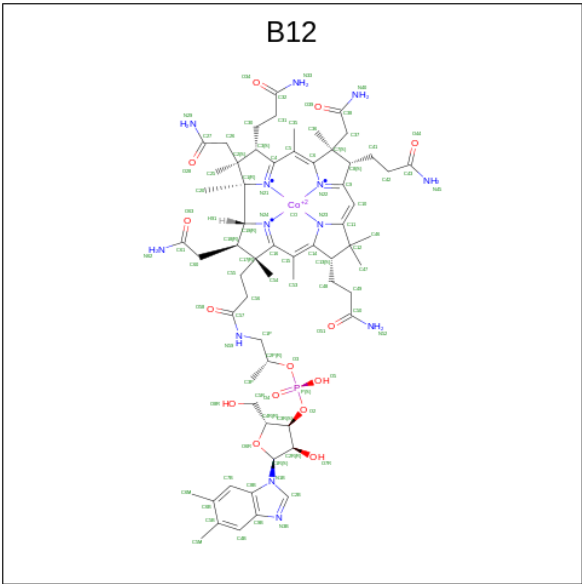
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Chain	Residue	Modelled	Actual	Comment	Reference
F	718	TRP	MET	engineered mutation	UNP O08505
G	556	GLN	-	linker	UNP Q59476
G	557	GLY	-	linker	UNP Q59476
G	558	GLY	-	linker	UNP Q59476
G	559	ILE	-	linker	UNP Q59476
G	560	PRO	-	linker	UNP Q59476
G	561	VAL	-	linker	UNP Q59476
G	718	TRP	MET	engineered mutation	UNP O08505

- Molecule 2 is a protein called Glycerol dehydrase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	137	Total	C	N	O	S	0	0	0
			1100	687	207	203	3			
2	E	139	Total	C	N	O	S	0	0	0
			1119	698	210	208	3			
2	H	140	Total	C	N	O	S	0	0	0
			1120	699	211	207	3			
2	I	141	Total	C	N	O	S	0	0	0
			1128	704	212	209	3			

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P) (labeled as "Lig- and of Interest" by depositor).



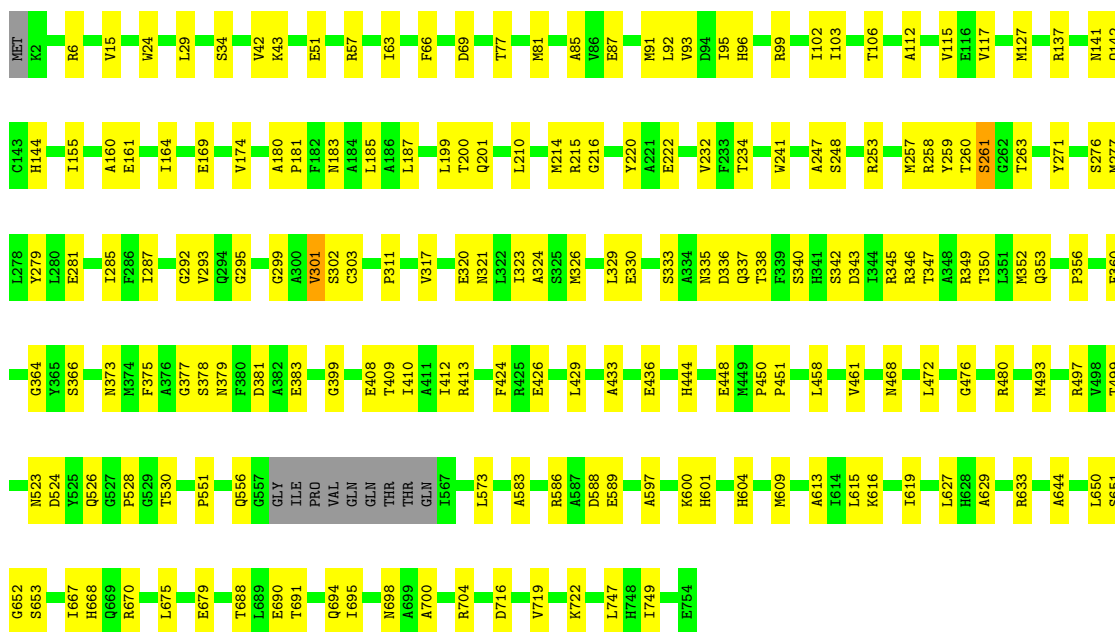
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	F	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	F	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

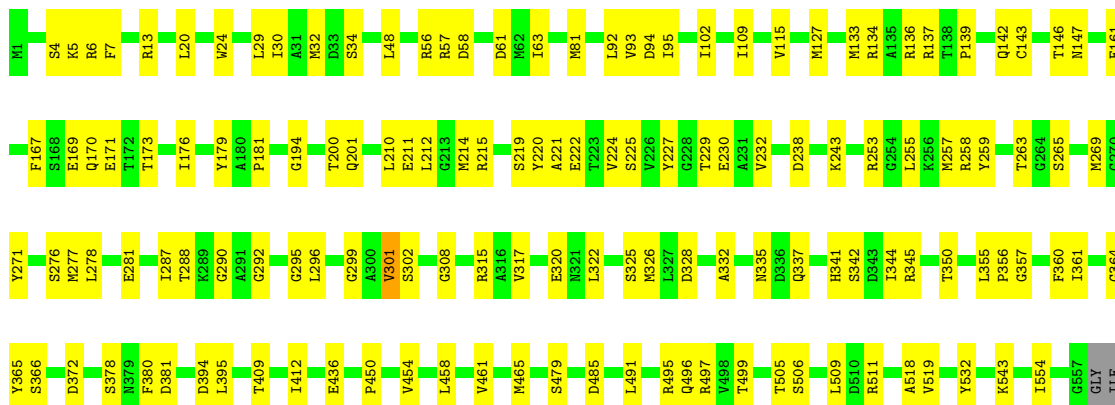
- Molecule 1: Glycerol dehydrase alpha subunit, Glycerol dehydrase beta subunit

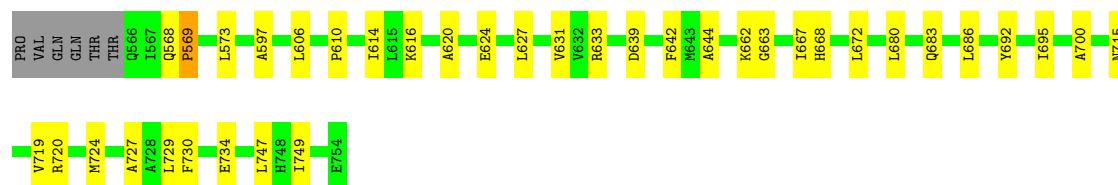
Chain B: 



- Molecule 1: Glycerol dehydrase alpha subunit, Glycerol dehydrase beta subunit

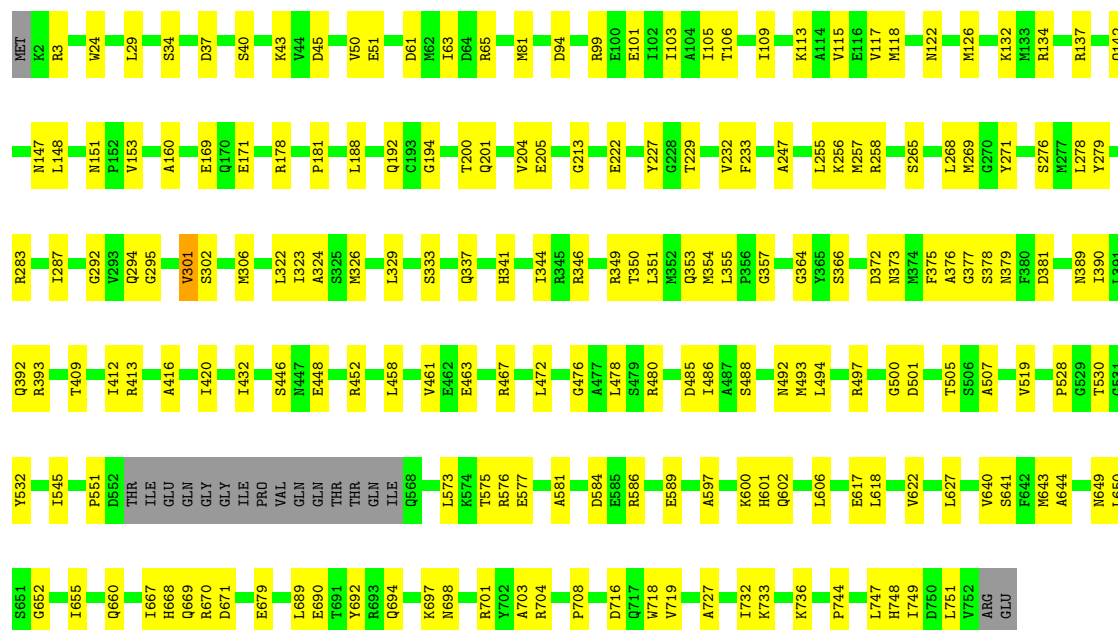
Chain C: 





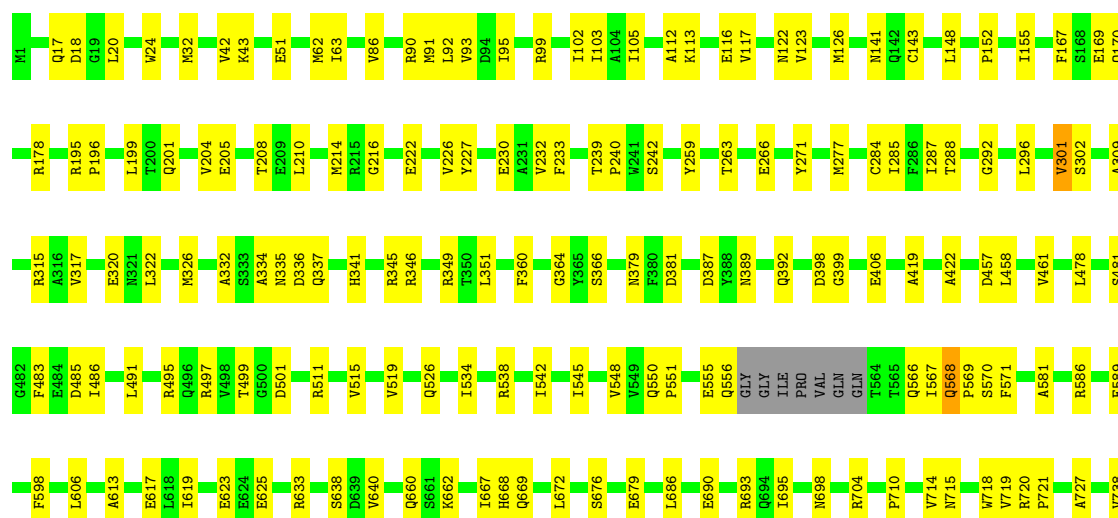
- Molecule 1: Glycerol dehydrase alpha subunit, Glycerol dehydrase beta subunit

Chain F: 72% 25% .



- Molecule 1: Glycerol dehydrase alpha subunit, Glycerol dehydrase beta subunit

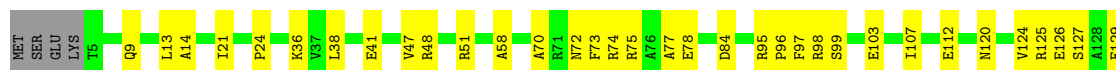
Chain G: 77% 22% .





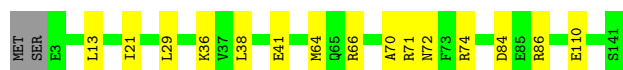
- Molecule 2: Glycerol dehydrase gamma subunit

Chain D: 71% 26% .



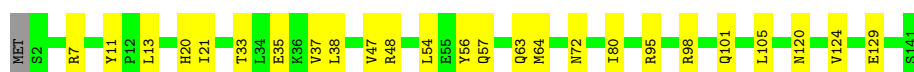
- Molecule 2: Glycerol dehydrase gamma subunit

Chain E: 88% 11% .



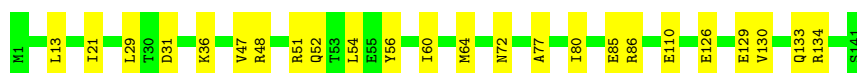
- Molecule 2: Glycerol dehydrase gamma subunit

Chain H: 82% 18% .



- Molecule 2: Glycerol dehydrase gamma subunit

Chain I: 83% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	153.55Å 155.57Å 381.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 3.68 29.99 – 3.68	Depositor EDS
% Data completeness (in resolution range)	92.1 (29.99-3.68) 88.7 (29.99-3.68)	Depositor EDS
R_{merge}	0.57	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 3.65Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.210 , 0.265 0.211 , 0.267	Depositor DCC
R_{free} test set	2299 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.064 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27597	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B12

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.16	0/5787	0.36	0/7841
1	C	0.18	0/5814	0.38	0/7875
1	F	0.13	0/5721	0.33	0/7752
1	G	0.14	0/5815	0.35	0/7879
2	D	0.15	0/1120	0.33	0/1518
2	E	0.12	0/1139	0.29	0/1541
2	H	0.13	0/1140	0.31	0/1544
2	I	0.11	0/1148	0.28	0/1555
All	All	0.15	0/27684	0.35	0/37505

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5694	0	5651	132	0
1	C	5721	0	5688	124	0
1	F	5629	0	5590	138	0
1	G	5722	0	5682	117	0
2	D	1100	0	1107	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1119	0	1126	14	0
2	H	1120	0	1127	18	0
2	I	1128	0	1133	17	0
3	B	91	0	87	6	0
3	C	91	0	87	8	0
3	F	182	0	174	25	0
All	All	27597	0	27452	549	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (549) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2601:B12:H421	3:F:2601:B12:C10	1.95	0.94
1:B:366:SER:HB3	1:B:381:ASP:HA	1.57	0.86
1:C:229:THR:OG1	1:C:232:VAL:HB	1.77	0.84
1:F:204:VAL:HG12	1:F:205:GLU:H	1.45	0.81
1:F:640:VAL:HB	1:F:660:GLN:HG3	1.64	0.79
1:B:675:LEU:HD13	3:B:2601:B12:H361	1.65	0.78
1:F:366:SER:HB3	1:F:381:ASP:HA	1.65	0.78
1:C:662:LYS:HG2	1:C:730:PHE:HB3	1.66	0.77
1:B:302:SER:HA	1:B:337:GLN:HG3	1.66	0.76
2:E:13:LEU:HB3	2:E:21:ILE:HD11	1.67	0.75
1:F:232:VAL:HG23	1:F:271:TYR:HB2	1.69	0.74
1:G:204:VAL:HG12	1:G:205:GLU:H	1.53	0.74
1:F:488:SER:O	1:F:492:ASN:ND2	2.20	0.74
1:C:232:VAL:HG13	1:C:269:MET:HE3	1.70	0.73
1:F:366:SER:HB2	1:F:378:SER:HB3	1.69	0.73
1:G:389:ASN:HA	1:G:392:GLN:HE21	1.53	0.72
1:G:586:ARG:HG3	1:G:589:GLU:HB3	1.72	0.72
1:G:690:GLU:OE1	1:G:693:ARG:NH1	2.24	0.71
1:C:142:GLN:HB2	1:C:169:GLU:HB2	1.73	0.71
1:G:288:THR:HG21	1:G:296:LEU:HD13	1.71	0.71
1:F:256:LYS:NZ	1:F:507:ALA:O	2.23	0.71
1:G:571:PHE:HB3	1:G:751:LEU:HD12	1.73	0.71
1:F:551:PRO:HG2	1:G:24:TRP:HB2	1.72	0.70
1:B:232:VAL:HG23	1:B:271:TYR:HB2	1.73	0.70
1:C:232:VAL:HG23	1:C:271:TYR:HB2	1.74	0.69
1:B:160:ALA:HB1	1:B:412:ILE:HG22	1.72	0.69
1:C:238:ASP:OD2	1:C:243:LYS:NZ	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:SER:HA	1:G:337:GLN:HG3	1.74	0.69
1:C:137:ARG:HG2	1:C:532:TYR:HB2	1.75	0.67
1:G:259:TYR:HD2	1:G:288:THR:HG22	1.59	0.67
1:C:292:GLY:HA3	2:E:72:ASN:HB2	1.77	0.67
2:H:13:LEU:HB3	2:H:21:ILE:HD11	1.77	0.67
1:G:112:ALA:O	1:G:116:GLU:HG3	1.94	0.66
1:C:573:LEU:HD12	1:C:749:ILE:HG23	1.77	0.66
1:B:321:ASN:OD1	1:B:353:GLN:NE2	2.28	0.66
1:B:352:MET:HE1	1:C:355:LEU:HD11	1.77	0.66
1:B:410:ILE:HD11	1:C:4:SER:HB2	1.77	0.66
1:C:290:GLY:O	2:E:71:ARG:NH2	2.29	0.66
1:C:301:VAL:HG13	1:C:302:SER:H	1.61	0.66
1:G:568:GLN:HB3	1:G:569:PRO:HD2	1.78	0.66
1:G:686:LEU:HD23	1:G:714:VAL:HB	1.78	0.65
1:B:556:GLN:O	1:B:604:HIS:NE2	2.30	0.65
1:F:178:ARG:HD2	1:F:458:LEU:HD13	1.79	0.65
1:B:303:CYS:HA	1:C:724:MET:HE1	1.79	0.64
1:C:63:ILE:HG23	1:C:287:ILE:HD11	1.80	0.64
1:B:337:GLN:HE22	1:B:375:PHE:HB3	1.63	0.64
1:F:341:HIS:CE1	1:G:718:TRP:HB3	2.33	0.64
1:C:161:GLU:HG3	1:C:409:THR:HG23	1.81	0.63
1:F:690:GLU:O	1:F:694:GLN:NE2	2.32	0.63
1:G:366:SER:HB3	1:G:381:ASP:HA	1.81	0.63
1:F:375:PHE:C	3:F:2601:B12:H622	2.07	0.63
1:G:216:GLY:HA2	1:G:497:ARG:HH22	1.64	0.63
1:F:265:SER:HB2	3:F:2601:B12:H471	1.80	0.63
1:F:268:LEU:HD22	3:F:2601:B12:H481	1.79	0.63
1:G:43:LYS:HB3	1:G:51:GLU:HB3	1.81	0.63
3:F:2601:B12:H421	3:F:2601:B12:H10	1.80	0.62
1:B:137:ARG:HG3	1:B:523:ASN:HA	1.82	0.62
1:B:722:LYS:HG3	1:C:341:HIS:CE1	2.34	0.62
1:C:181:PRO:HB3	1:C:212:LEU:HD21	1.80	0.62
1:F:530:THR:HG23	1:G:90:ARG:HH22	1.64	0.62
1:G:62:MET:HG3	2:I:134:ARG:HG3	1.82	0.62
3:F:2601:B12:H1P1	1:G:719:VAL:HG12	1.82	0.62
1:G:91:MET:HE1	1:G:105:ILE:HD12	1.81	0.61
1:B:263:THR:HB	1:B:277:MET:HB3	1.81	0.61
1:G:292:GLY:HA3	2:I:72:ASN:HB2	1.81	0.61
2:D:51:ARG:HD2	2:D:77:ALA:HB1	1.82	0.61
1:B:651:SER:O	1:B:670:ARG:NH2	2.33	0.61
1:F:390:ILE:HD13	1:F:545:ILE:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LYS:HB3	1:B:51:GLU:HB3	1.82	0.61
1:F:192:GLN:HE22	1:F:493:MET:HE3	1.66	0.61
1:F:346:ARG:NH2	1:F:350:THR:OG1	2.33	0.60
3:F:2601:B12:C10	3:F:2601:B12:C42	2.75	0.60
1:F:617:GLU:HG3	1:F:689:LEU:HB3	1.83	0.60
1:F:333:SER:HB2	1:F:353:GLN:HG2	1.83	0.60
2:H:95:ARG:HB2	2:H:98:ARG:HG3	1.83	0.60
2:D:78:GLU:OE1	2:D:120:ASN:ND2	2.35	0.59
1:F:472:LEU:HD22	2:H:37:VAL:HG11	1.83	0.59
1:G:679:GLU:OE2	1:G:698:ASN:ND2	2.35	0.59
1:B:210:LEU:HD21	1:B:214:MET:HE3	1.84	0.59
2:E:64:MET:HB3	2:E:66:ARG:HH11	1.67	0.59
1:F:346:ARG:NH1	1:F:346:ARG:O	2.35	0.59
1:C:127:MET:HG2	1:C:356:PRO:HG3	1.84	0.59
1:C:139:PRO:HB2	1:C:361:ILE:HD11	1.82	0.59
1:C:302:SER:HA	1:C:337:GLN:HG3	1.83	0.59
1:F:494:LEU:HB3	2:H:47:VAL:HG11	1.85	0.59
1:G:263:THR:HB	1:G:277:MET:HB3	1.84	0.59
1:B:57:ARG:NH2	1:B:69:ASP:OD1	2.36	0.59
1:B:383:GLU:O	1:C:13:ARG:HD2	2.03	0.59
1:G:619:ILE:O	1:G:623:GLU:HG3	2.03	0.59
1:C:134:ARG:NH1	1:C:357:GLY:O	2.35	0.58
1:B:526:GLN:H	1:B:530:THR:HG1	1.51	0.58
2:D:36:LYS:NZ	2:D:41:GLU:OE1	2.30	0.58
1:F:65:ARG:NH2	2:H:129:GLU:OE2	2.35	0.58
1:C:465:MET:HE2	1:C:465:MET:HA	1.86	0.58
3:F:2601:B12:H621	1:G:720:ARG:HH12	1.51	0.58
1:B:690:GLU:O	1:B:694:GLN:HG2	2.04	0.58
1:B:722:LYS:HG3	1:C:341:HIS:HE1	1.68	0.58
3:F:2601:B12:H4R	3:F:2601:B12:H551	1.86	0.57
1:B:63:ILE:HG23	1:B:287:ILE:HD11	1.85	0.57
1:B:433:ALA:HB3	1:B:436:GLU:HG3	1.87	0.57
1:C:56:ARG:NH1	1:C:58:ASP:OD2	2.38	0.57
1:B:261:SER:OG	1:B:281:GLU:OE2	2.23	0.57
1:G:478:LEU:HD22	1:G:486:ILE:HD11	1.85	0.57
1:B:424:PHE:HA	1:B:429:LEU:HD12	1.87	0.57
1:C:332:ALA:HA	1:C:360:PHE:HB2	1.87	0.57
1:G:550:GLN:HG2	1:G:551:PRO:HD2	1.85	0.57
1:G:718:TRP:HA	1:G:721:PRO:HG2	1.84	0.57
1:G:478:LEU:HD13	1:G:486:ILE:HG13	1.86	0.56
1:B:444:HIS:O	1:C:6:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:640:VAL:HA	1:F:643:MET:HE2	1.85	0.56
1:B:164:ILE:HG21	1:B:412:ILE:HG13	1.87	0.56
1:B:292:GLY:HA3	2:D:72:ASN:HB2	1.87	0.56
1:C:366:SER:HB3	1:C:381:ASP:HA	1.87	0.56
1:F:586:ARG:HG3	1:F:589:GLU:HB3	1.86	0.56
1:B:323:ILE:HA	1:B:326:MET:HG2	1.86	0.56
1:F:597:ALA:HB1	1:F:601:HIS:HB2	1.87	0.56
1:B:633:ARG:HB2	1:B:747:LEU:HD11	1.88	0.56
1:C:436:GLU:HG2	1:C:450:PRO:HG2	1.86	0.56
1:C:20:LEU:HD21	1:C:345:ARG:HH12	1.70	0.56
1:G:485:ASP:OD1	1:G:485:ASP:N	2.39	0.56
1:F:694:GLN:HA	1:F:697:LYS:HG3	1.88	0.56
1:B:589:GLU:O	1:B:653:SER:OG	2.22	0.56
2:H:120:ASN:O	2:H:124:VAL:HG23	2.06	0.56
1:B:350:THR:OG1	1:B:379:ASN:ND2	2.39	0.55
3:F:2601:B12:C10	3:F:2601:B12:H482	2.35	0.55
1:F:641:SER:HB2	3:F:2602:B12:HM61	1.88	0.55
1:F:716:ASP:HB3	1:F:719:VAL:HG23	1.87	0.55
1:B:627:LEU:HD13	1:B:700:ALA:HB1	1.88	0.55
1:B:161:GLU:OE1	1:B:413:ARG:NH1	2.40	0.55
1:F:718:TRP:HB3	1:G:341:HIS:HE1	1.71	0.55
1:B:499:THR:HG21	2:D:14:ALA:HB2	1.89	0.55
1:B:338:THR:H	1:C:720:ARG:HH21	1.54	0.55
3:B:2601:B12:H471	1:C:265:SER:HB2	1.89	0.55
1:B:144:HIS:CE1	1:B:336:ASP:HB2	2.42	0.55
2:I:86:ARG:NH1	2:I:110:GLU:OE1	2.40	0.55
1:C:225:SER:O	1:C:243:LYS:HE2	2.07	0.54
1:F:351:LEU:HD23	1:F:354:MET:HE3	1.88	0.54
1:G:216:GLY:HA2	1:G:497:ARG:NH2	2.22	0.54
1:C:146:THR:HG21	1:C:173:THR:HG22	1.89	0.54
1:G:232:VAL:HG23	1:G:271:TYR:HB2	1.89	0.54
1:B:613:ALA:HA	1:B:616:LYS:HE2	1.89	0.54
1:B:142:GLN:HB2	1:B:169:GLU:HB2	1.89	0.54
1:F:99:ARG:O	1:F:103:ILE:HG12	2.07	0.54
1:G:210:LEU:O	1:G:214:MET:HG3	2.08	0.54
2:I:126:GLU:O	2:I:130:VAL:HG23	2.07	0.54
1:C:355:LEU:HD21	1:C:395:LEU:HD13	1.90	0.54
1:B:627:LEU:HD11	1:B:704:ARG:HG3	1.90	0.54
1:C:115:VAL:HG12	1:C:278:LEU:HG	1.90	0.54
1:C:211:GLU:OE2	1:C:215:ARG:NH1	2.41	0.54
1:G:491:LEU:O	1:G:495:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ASN:ND2	1:B:399:GLY:O	2.41	0.54
1:C:143:CYS:SG	1:C:170:GLN:HG2	2.48	0.54
1:G:336:ASP:O	1:G:337:GLN:NE2	2.26	0.53
1:C:220:TYR:CE2	1:C:222:GLU:HB2	2.43	0.53
1:C:255:LEU:HD21	1:C:497:ARG:CZ	2.38	0.53
1:F:118:MET:HG3	1:F:323:ILE:HD11	1.90	0.53
1:B:320:GLU:HA	1:B:323:ILE:HG22	1.89	0.53
1:B:333:SER:HB2	1:B:353:GLN:HG2	1.89	0.53
1:F:337:GLN:HE22	1:F:375:PHE:HB3	1.73	0.53
1:F:458:LEU:O	1:F:461:VAL:HG12	2.08	0.53
1:B:42:VAL:HG11	1:B:77:THR:HG22	1.89	0.53
1:B:373:ASN:HB3	1:B:377:GLY:HA2	1.91	0.53
1:C:179:TYR:OH	1:C:454:VAL:HG13	2.08	0.53
1:C:210:LEU:HD21	1:C:214:MET:HE3	1.91	0.53
2:E:36:LYS:NZ	2:E:41:GLU:OE1	2.40	0.53
2:D:103:GLU:O	2:D:107:ILE:HG12	2.09	0.53
1:F:302:SER:HA	1:F:337:GLN:HG3	1.91	0.53
1:F:581:ALA:HB3	1:F:744:PRO:HB2	1.89	0.53
1:B:85:ALA:HB1	1:B:117:VAL:HA	1.89	0.53
1:B:426:GLU:OE1	1:B:480:ARG:NH1	2.37	0.53
2:D:95:ARG:HB2	2:D:98:ARG:HG3	1.91	0.53
1:F:204:VAL:HG12	1:F:205:GLU:N	2.21	0.53
1:B:199:LEU:HD23	1:B:493:MET:HE1	1.91	0.53
1:B:573:LEU:HD21	1:B:749:ILE:HG23	1.90	0.53
1:B:615:LEU:O	1:B:619:ILE:HG13	2.09	0.53
1:B:6:ARG:NH1	1:C:161:GLU:OE1	2.42	0.52
1:F:337:GLN:HA	1:F:337:GLN:HE21	1.74	0.52
1:F:351:LEU:HD12	1:G:351:LEU:HD12	1.91	0.52
1:G:266:GLU:OE1	1:G:266:GLU:N	2.42	0.52
2:I:13:LEU:HD12	2:I:21:ILE:HD11	1.92	0.52
1:C:610:PRO:O	1:C:614:ILE:HG12	2.09	0.52
1:C:627:LEU:HD13	1:C:700:ALA:HB1	1.91	0.52
1:G:204:VAL:HG12	1:G:205:GLU:N	2.21	0.52
1:C:519:VAL:HG22	2:E:64:MET:HG3	1.91	0.52
1:F:373:ASN:HB3	1:F:377:GLY:HA2	1.91	0.52
1:F:732:ILE:O	1:F:736:LYS:HG2	2.08	0.52
1:G:457:ASP:O	1:G:461:VAL:HG23	2.10	0.52
1:C:308:GLY:O	1:C:345:ARG:NH2	2.42	0.52
1:F:115:VAL:HG12	1:F:278:LEU:HG	1.92	0.52
1:F:644:ALA:HB1	1:F:668:HIS:HB2	1.92	0.52
1:G:640:VAL:HB	1:G:660:GLN:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:31:ASP:OD1	2:I:36:LYS:NZ	2.41	0.52
1:F:188:LEU:HA	1:F:200:THR:HG21	1.92	0.51
2:H:33:THR:O	2:H:37:VAL:HG23	2.11	0.51
1:C:176:ILE:HB	1:C:179:TYR:HD2	1.73	0.51
1:F:409:THR:O	1:F:413:ARG:HG3	2.10	0.51
1:G:17:GLN:HB2	1:G:341:HIS:CD2	2.45	0.51
2:I:129:GLU:O	2:I:133:GLN:HG3	2.10	0.51
2:D:24:PRO:HG3	2:D:48:ARG:HB2	1.92	0.51
1:B:259:TYR:CE1	1:B:293:VAL:HG21	2.46	0.51
1:B:346:ARG:HB2	1:B:379:ASN:OD1	2.11	0.51
1:B:476:GLY:HA2	2:D:38:LEU:HD21	1.92	0.51
1:F:575:THR:HB	1:F:747:LEU:HD22	1.92	0.51
1:F:618:LEU:O	1:F:622:VAL:HG23	2.11	0.51
2:D:112:GLU:OE1	2:D:125:ARG:NH2	2.40	0.51
1:B:253:ARG:NH2	2:D:84:ASP:OD1	2.42	0.51
1:C:143:CYS:HB3	1:C:167:PHE:CD1	2.46	0.51
1:F:701:ARG:HD2	1:F:708:PRO:HB3	1.92	0.51
1:B:472:LEU:HD11	2:D:47:VAL:HG21	1.92	0.51
1:G:196:PRO:HG2	1:G:511:ARG:HG3	1.92	0.51
1:B:222:GLU:OE2	1:B:258:ARG:NH1	2.44	0.51
1:B:222:GLU:O	1:B:260:THR:OG1	2.27	0.51
1:B:589:GLU:OE2	1:B:652:GLY:N	2.38	0.51
1:C:667:ILE:HD11	1:C:695:ILE:HG23	1.92	0.51
1:G:284:CYS:O	1:G:288:THR:HG23	2.11	0.51
1:B:142:GLN:NE2	1:B:169:GLU:OE1	2.44	0.51
1:C:142:GLN:NE2	1:C:171:GLU:OE1	2.43	0.51
1:C:224:VAL:HG21	1:C:257:MET:HE2	1.93	0.50
2:D:9:GLN:OE1	2:D:9:GLN:N	2.38	0.50
1:B:24:TRP:HB3	1:B:29:LEU:HB2	1.92	0.50
1:C:496:GLN:HG3	1:C:509:LEU:HD11	1.93	0.50
3:F:2602:B12:C5	3:F:2602:B12:H4B	2.41	0.50
1:G:86:VAL:O	1:G:90:ARG:HG3	2.11	0.50
1:G:317:VAL:O	1:G:320:GLU:HG2	2.11	0.50
1:C:200:THR:H	1:C:219:SER:HB2	1.75	0.50
1:F:24:TRP:HB2	1:G:551:PRO:HG2	1.92	0.50
1:F:718:TRP:HB3	1:G:341:HIS:CE1	2.46	0.50
1:G:259:TYR:CD2	1:G:288:THR:HG22	2.43	0.50
1:C:288:THR:HG21	1:C:296:LEU:HB2	1.93	0.50
1:C:631:VAL:HG12	1:C:747:LEU:HD12	1.93	0.50
1:C:299:GLY:C	1:C:301:VAL:H	2.19	0.50
2:I:85:GLU:CD	2:I:85:GLU:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:VAL:HG11	1:B:279:TYR:HA	1.94	0.49
1:C:253:ARG:NH2	2:E:84:ASP:OD1	2.34	0.49
1:F:137:ARG:HG2	1:F:532:TYR:HB2	1.94	0.49
1:F:393:ARG:HD2	1:F:545:ILE:HD12	1.93	0.49
1:F:113:LYS:O	1:F:117:VAL:HG23	2.13	0.49
1:C:505:THR:HB	1:C:518:ALA:HB3	1.94	0.49
1:F:148:LEU:N	1:F:372:ASP:OD1	2.44	0.49
1:C:81:MET:HE1	1:C:109:ILE:HA	1.95	0.49
1:C:614:ILE:HD12	1:C:692:TYR:CE2	2.48	0.49
1:F:463:GLU:O	1:F:467:ARG:N	2.39	0.49
1:B:347:THR:OG1	1:C:344:ILE:HG13	2.13	0.49
3:B:2601:B12:C11	3:B:2601:B12:H491	2.43	0.49
1:C:221:ALA:O	1:C:257:MET:HA	2.13	0.49
1:C:302:SER:HA	1:C:337:GLN:HE21	1.78	0.49
1:C:499:THR:HG22	2:E:29:LEU:HD11	1.95	0.49
1:F:232:VAL:HG13	1:F:269:MET:HE2	1.95	0.49
1:B:216:GLY:HA2	1:B:497:ARG:NH2	2.28	0.49
1:B:241:TRP:CD1	2:D:127:SER:HB3	2.48	0.49
1:B:311:PRO:HG3	1:C:543:LYS:HD2	1.94	0.49
2:I:54:LEU:HD12	2:I:80:ILE:HD11	1.95	0.49
1:B:597:ALA:HB1	1:B:601:HIS:HB2	1.95	0.49
1:B:96:HIS:NE2	1:C:94:ASP:OD2	2.46	0.48
2:H:20:HIS:HB3	2:H:56:TYR:HE2	1.78	0.48
1:C:61:ASP:HB2	1:C:230:GLU:OE2	2.14	0.48
1:F:301:VAL:HG12	1:F:302:SER:N	2.29	0.48
1:F:142:GLN:HG3	1:F:169:GLU:HB2	1.95	0.48
1:G:239:THR:H	1:G:242:SER:HG	1.62	0.48
1:C:683:GLN:NE2	1:C:715:ASN:OD1	2.43	0.48
1:F:160:ALA:HB2	1:F:416:ALA:HB2	1.95	0.48
1:F:247:ALA:HA	1:F:257:MET:HE3	1.93	0.48
3:F:2601:B12:HM63	1:G:640:VAL:HG13	1.95	0.48
1:C:511:ARG:HH11	1:C:511:ARG:HB3	1.78	0.48
2:I:48:ARG:HH12	2:I:80:ILE:HG23	1.78	0.48
1:B:258:ARG:HB2	1:B:295:GLY:C	2.39	0.48
1:F:337:GLN:NE2	1:F:375:PHE:O	2.41	0.48
1:F:448:GLU:N	1:F:448:GLU:OE1	2.46	0.48
1:F:501:ASP:O	2:H:11:TYR:OH	2.31	0.48
1:F:649:ASN:HA	1:F:670:ARG:HG3	1.94	0.48
1:G:567:ILE:HD13	1:G:570:SER:OG	2.13	0.48
3:B:2601:B12:H291	3:B:2601:B12:C19	2.26	0.48
1:F:606:LEU:HD21	1:F:727:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:PRO:HA	1:G:155:ILE:HD12	1.95	0.48
1:F:372:ASP:OD2	1:F:446:SER:N	2.46	0.48
1:F:389:ASN:HA	1:F:392:GLN:HE21	1.78	0.48
1:G:322:LEU:O	1:G:326:MET:HG2	2.13	0.48
1:B:95:ILE:HD13	1:C:93:VAL:HG23	1.95	0.48
1:B:679:GLU:OE2	1:B:698:ASN:ND2	2.42	0.48
1:B:317:VAL:O	1:B:320:GLU:HG2	2.14	0.47
1:B:366:SER:HB2	1:B:378:SER:HB3	1.95	0.47
1:F:478:LEU:HD13	1:F:486:ILE:HG22	1.95	0.47
1:B:99:ARG:O	1:B:103:ILE:HG12	2.14	0.47
1:C:201:GLN:NE2	1:C:222:GLU:HB3	2.29	0.47
1:F:337:GLN:NE2	1:F:375:PHE:HB3	2.28	0.47
1:B:526:GLN:N	1:B:530:THR:OG1	2.35	0.47
1:F:63:ILE:HG12	1:F:287:ILE:HD11	1.95	0.47
1:C:136:ARG:HE	1:C:506:SER:HB3	1.79	0.47
1:C:147:ASN:HA	1:C:372:ASP:HB3	1.95	0.47
1:C:366:SER:HB2	1:C:378:SER:HB3	1.95	0.47
1:G:545:ILE:O	1:G:548:VAL:HG22	2.15	0.47
3:C:2601:B12:H412	3:C:2601:B12:H363	1.40	0.47
1:F:485:ASP:OD1	1:F:485:ASP:N	2.39	0.47
1:G:148:LEU:HD23	1:G:148:LEU:HA	1.79	0.47
1:F:122:ASN:O	1:F:126:MET:HG3	2.15	0.47
2:H:54:LEU:HD12	2:H:80:ILE:HD11	1.96	0.47
1:B:343:ASP:CG	1:B:346:ARG:HH21	2.23	0.47
1:G:143:CYS:HB3	1:G:167:PHE:CD1	2.50	0.47
2:H:7:ARG:HA	2:H:63:GLN:HG2	1.97	0.47
2:I:48:ARG:HH22	2:I:80:ILE:HG22	1.79	0.47
2:E:70:ALA:O	2:E:74:ARG:HG3	2.14	0.47
1:F:24:TRP:HB3	1:F:29:LEU:HD12	1.96	0.47
1:F:301:VAL:HG12	1:F:302:SER:H	1.79	0.47
1:F:667:ILE:HD12	1:F:679:GLU:HB2	1.97	0.47
1:C:511:ARG:HB3	1:C:511:ARG:NH1	2.30	0.47
2:E:64:MET:HB3	2:E:66:ARG:NH1	2.30	0.47
1:F:655:ILE:HG13	1:F:703:ALA:HA	1.97	0.47
1:B:247:ALA:HA	1:B:257:MET:HE3	1.96	0.46
1:B:586:ARG:O	1:B:652:GLY:HA3	2.15	0.46
1:B:667:ILE:HD11	1:B:695:ILE:HG23	1.95	0.46
1:C:263:THR:HG22	1:C:281:GLU:HB2	1.97	0.46
2:D:126:GLU:O	2:D:130:VAL:HG23	2.14	0.46
1:C:181:PRO:HG2	1:C:461:VAL:CG2	2.46	0.46
1:F:147:ASN:HD21	1:F:151:ASN:H	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:ILE:HG23	1:G:287:ILE:HD11	1.96	0.46
1:G:581:ALA:HB3	1:G:744:PRO:HB2	1.98	0.46
1:G:669:GLN:HB3	1:G:672:LEU:HD13	1.96	0.46
1:B:93:VAL:HG23	1:C:95:ILE:HD13	1.95	0.46
1:F:322:LEU:O	1:F:326:MET:HG2	2.16	0.46
3:F:2601:B12:C16	3:F:2601:B12:H2B	2.46	0.46
3:F:2602:B12:HM61	3:F:2602:B12:HM53	1.64	0.46
1:G:301:VAL:HG12	1:G:302:SER:N	2.30	0.46
1:B:551:PRO:HG3	1:C:24:TRP:HB2	1.97	0.46
1:F:476:GLY:O	1:F:480:ARG:HG3	2.15	0.46
1:B:458:LEU:O	1:B:461:VAL:HG12	2.14	0.46
1:B:586:ARG:O	1:B:589:GLU:HG2	2.15	0.46
1:B:675:LEU:HD22	3:B:2601:B12:H411	1.97	0.46
1:G:99:ARG:O	1:G:103:ILE:HG12	2.14	0.46
1:B:15:VAL:HB	1:B:342:SER:HB2	1.98	0.46
1:B:87:GLU:O	1:B:91:MET:HG3	2.15	0.46
3:F:2602:B12:H482	3:F:2602:B12:H473	1.15	0.46
3:F:2602:B12:H531	3:F:2602:B12:H552	1.96	0.46
1:G:606:LEU:HD21	1:G:727:ALA:HA	1.97	0.46
1:F:3:ARG:HH11	1:G:406:GLU:CD	2.24	0.46
1:F:229:THR:O	1:F:233:PHE:HB2	2.16	0.46
1:F:355:LEU:HD22	1:G:123:VAL:HG21	1.97	0.46
3:F:2601:B12:H492	3:F:2601:B12:H533	1.98	0.46
1:F:500:GLY:O	2:H:57:GLN:NE2	2.49	0.46
1:C:633:ARG:HB2	1:C:747:LEU:HD21	1.98	0.46
1:B:345:ARG:NH2	1:C:394:ASP:OD2	2.47	0.46
1:C:48:LEU:HD21	1:C:57:ARG:NE	2.31	0.46
1:F:34:SER:HB2	1:F:276:SER:HB3	1.98	0.46
1:F:573:LEU:HD21	1:F:749:ILE:HD12	1.98	0.46
1:G:419:ALA:HA	1:G:483:PHE:CE2	2.51	0.46
2:D:99:SER:HB3	2:D:103:GLU:HB2	1.98	0.45
1:B:526:GLN:HB2	1:B:530:THR:HG21	1.99	0.45
1:B:201:GLN:HE22	1:B:222:GLU:HB3	1.81	0.45
1:G:613:ALA:O	1:G:617:GLU:HG2	2.16	0.45
1:F:393:ARG:NH1	1:G:20:LEU:HD12	2.31	0.45
1:F:602:GLN:OE1	1:F:733:LYS:HB3	2.17	0.45
1:G:660:GLN:OE1	1:G:662:LYS:HE3	2.16	0.45
1:F:279:TYR:CE2	1:F:283:ARG:HD2	2.52	0.45
1:B:127:MET:HG2	1:B:356:PRO:HG3	1.97	0.45
1:C:30:ILE:O	1:C:277:MET:HG3	2.17	0.45
1:F:134:ARG:NH1	1:F:357:GLY:O	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:301:VAL:HG22	1:G:334:ALA:HB2	1.97	0.45
1:F:94:ASP:O	1:F:132:LYS:NZ	2.45	0.45
1:F:376:ALA:HB3	1:G:720:ARG:NH2	2.31	0.45
1:F:618:LEU:HD12	1:F:692:TYR:HB3	1.99	0.45
3:F:2602:B12:H311	3:F:2602:B12:H352	1.98	0.45
1:G:332:ALA:HA	1:G:360:PHE:HB2	1.98	0.44
1:G:686:LEU:CD1	1:G:719:VAL:HG21	2.47	0.44
1:B:285:ILE:HD13	1:B:323:ILE:HG23	1.99	0.44
1:F:43:LYS:HB3	1:F:51:GLU:HB3	1.99	0.44
1:G:227:TYR:CD2	1:G:233:PHE:HA	2.52	0.44
2:H:35:GLU:HA	2:H:38:LEU:HD12	1.99	0.44
3:F:2601:B12:H10	3:F:2601:B12:C42	2.43	0.44
1:G:32:MET:SD	1:G:315:ARG:NH1	2.90	0.44
1:G:62:MET:SD	1:G:240:PRO:HD2	2.57	0.44
1:G:422:ALA:HB1	1:G:481:SER:HB2	1.98	0.44
1:G:205:GLU:OE1	1:G:208:THR:HG23	2.17	0.44
1:F:61:ASP:OD1	1:F:61:ASP:N	2.50	0.44
1:F:351:LEU:HD22	1:F:355:LEU:HG	2.00	0.44
1:F:577:GLU:OE2	1:F:600:LYS:HE2	2.17	0.44
1:B:201:GLN:NE2	1:B:222:GLU:HB3	2.33	0.44
3:C:2601:B12:H541	3:C:2601:B12:H561	1.55	0.44
1:F:528:PRO:HD3	1:G:93:VAL:HG21	2.00	0.44
1:F:627:LEU:HD11	1:F:704:ARG:HG2	1.99	0.44
1:G:226:VAL:HG23	1:G:284:CYS:HB3	1.98	0.44
1:G:398:ASP:N	1:G:534:ILE:HD11	2.32	0.44
1:B:34:SER:HB2	1:B:276:SER:HB3	1.99	0.44
3:C:2601:B12:H491	3:C:2601:B12:H473	2.00	0.44
3:F:2602:B12:H602	3:F:2602:B12:H541	1.62	0.44
1:B:160:ALA:O	1:B:164:ILE:HG23	2.17	0.44
1:B:619:ILE:HG23	1:B:629:ALA:HB3	2.00	0.44
1:B:716:ASP:HB3	1:B:719:VAL:HG23	1.99	0.44
2:D:129:GLU:O	2:D:133:GLN:HG3	2.18	0.44
1:F:258:ARG:HB2	1:F:295:GLY:C	2.43	0.44
1:F:733:LYS:HD3	1:F:733:LYS:HA	1.86	0.44
1:G:519:VAL:HA	2:I:64:MET:HE2	1.99	0.44
3:B:2601:B12:H301	3:B:2601:B12:H253	1.54	0.44
1:F:3:ARG:HD3	1:G:406:GLU:OE2	2.18	0.44
1:C:680:LEU:HD11	3:C:2601:B12:HM62	2.00	0.43
2:D:70:ALA:O	2:D:74:ARG:HG3	2.18	0.43
1:F:40:SER:HB2	1:F:81:MET:HE1	2.00	0.43
1:F:153:VAL:HG22	1:F:432:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:373:ASN:O	1:G:715:ASN:ND2	2.51	0.43
3:F:2601:B12:C36	3:F:2601:B12:H351	2.48	0.43
1:G:538:ARG:O	1:G:542:ILE:HG13	2.18	0.43
1:C:24:TRP:HB3	1:C:29:LEU:HB2	1.99	0.43
1:C:322:LEU:O	1:C:326:MET:HG2	2.18	0.43
1:C:342:SER:OG	1:C:344:ILE:HG22	2.18	0.43
1:G:499:THR:HG22	2:I:29:LEU:HD21	1.99	0.43
1:C:32:MET:SD	1:C:315:ARG:NH1	2.91	0.43
1:C:258:ARG:HB2	1:C:295:GLY:C	2.43	0.43
1:F:584:ASP:OD1	1:F:652:GLY:HA2	2.18	0.43
1:C:554:ILE:HG21	1:C:729:LEU:HD13	2.00	0.43
1:F:106:THR:O	1:F:109:ILE:HG12	2.18	0.43
1:G:169:GLU:HG2	1:G:199:LEU:HB2	2.00	0.43
1:B:102:ILE:O	1:B:106:THR:HG23	2.18	0.43
1:C:34:SER:HB2	1:C:276:SER:HB3	2.00	0.43
1:C:222:GLU:HG2	1:C:258:ARG:HG2	2.00	0.43
1:F:147:ASN:HD21	1:F:151:ASN:N	2.16	0.43
1:G:667:ILE:HD11	1:G:695:ILE:HG23	1.99	0.43
2:I:56:TYR:O	2:I:60:ILE:HG12	2.19	0.43
1:B:317:VAL:HG11	1:B:349:ARG:HH21	1.83	0.43
1:C:573:LEU:HD23	1:C:616:LYS:HB2	2.01	0.43
1:C:639:ASP:HB3	1:C:642:PHE:HD2	1.83	0.43
1:F:349:ARG:HD2	1:F:379:ASN:ND2	2.34	0.43
1:F:432:ILE:HG12	1:F:452:ARG:HH12	1.83	0.43
1:G:178:ARG:NH1	1:G:458:LEU:HD13	2.33	0.43
1:C:485:ASP:OD1	1:C:485:ASP:N	2.51	0.43
3:C:2601:B12:H203	3:C:2601:B12:H253	1.71	0.43
1:F:101:GLU:O	1:F:105:ILE:HG13	2.18	0.43
1:G:42:VAL:HA	1:G:51:GLU:O	2.19	0.43
1:B:92:LEU:HD23	1:B:102:ILE:HD13	2.01	0.43
1:B:324:ALA:O	1:B:329:LEU:HB2	2.18	0.43
1:C:92:LEU:HD23	1:C:102:ILE:HD13	2.01	0.43
1:C:259:TYR:HB2	1:C:288:THR:HG23	2.01	0.43
1:C:606:LEU:HD11	1:C:727:ALA:HB2	1.99	0.43
1:B:174:VAL:HG11	1:B:180:ALA:HA	2.01	0.42
1:F:292:GLY:HA3	2:H:72:ASN:HB2	2.01	0.42
1:G:92:LEU:HD23	1:G:102:ILE:HD13	2.01	0.42
1:G:335:ASN:HA	1:G:349:ARG:NH1	2.34	0.42
1:C:133:MET:HB3	1:C:325:SER:HB3	2.00	0.42
1:C:227:TYR:HB3	1:C:232:VAL:HG12	2.01	0.42
1:C:568:GLN:O	1:C:569:PRO:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:CYS:SG	1:G:170:GLN:HG2	2.59	0.42
1:G:638:SER:HB3	1:G:738:VAL:CG2	2.50	0.42
2:H:64:MET:HE2	2:H:64:MET:HA	2.00	0.42
1:B:408:GLU:O	1:B:412:ILE:HG12	2.19	0.42
1:B:448:GLU:OE2	1:C:5:LYS:HD3	2.18	0.42
1:C:686:LEU:HD11	1:C:719:VAL:HG21	2.01	0.42
1:F:751:LEU:HD12	1:F:751:LEU:HA	1.83	0.42
1:G:346:ARG:HB2	1:G:379:ASN:OD1	2.19	0.42
2:I:51:ARG:HG2	2:I:77:ALA:HB1	2.00	0.42
1:B:187:LEU:HD23	1:B:200:THR:HB	2.01	0.42
1:B:528:PRO:CD	1:C:93:VAL:HG21	2.49	0.42
1:F:29:LEU:HD22	1:F:306:MET:HE1	2.02	0.42
1:B:169:GLU:HG3	1:B:360:PHE:CE1	2.55	0.42
1:B:609:MET:HE1	1:B:688:THR:HA	2.01	0.42
1:C:194:GLY:HA2	1:C:412:ILE:HG12	2.01	0.42
1:C:479:SER:OG	2:E:38:LEU:HD21	2.20	0.42
1:C:495:ARG:NH2	2:E:29:LEU:HD22	2.35	0.42
2:D:13:LEU:HD23	2:D:21:ILE:HD11	2.01	0.42
1:F:222:GLU:HG3	1:F:258:ARG:HD2	2.01	0.42
3:F:2601:B12:H482	3:F:2601:B12:H473	1.25	0.42
1:G:195:ARG:NH1	1:G:196:PRO:O	2.52	0.42
1:B:373:ASN:O	1:C:715:ASN:ND2	2.52	0.42
1:C:335:ASN:OD1	1:C:350:THR:HA	2.20	0.42
1:F:337:GLN:N	1:F:379:ASN:HB2	2.34	0.42
1:G:141:ASN:ND2	1:G:399:GLY:O	2.52	0.42
1:G:501:ASP:HB3	1:G:515:VAL:HG21	2.01	0.42
1:C:458:LEU:HA	1:C:461:VAL:HG12	2.01	0.42
3:C:2601:B12:H2B	3:C:2601:B12:C15	2.50	0.42
1:F:346:ARG:HH22	1:F:350:THR:HG1	1.66	0.42
1:F:650:LEU:HD11	1:F:744:PRO:HG3	2.02	0.42
1:G:555:GLU:HG3	1:G:556:GLN:N	2.35	0.42
1:B:295:GLY:HA2	1:B:330:GLU:HB3	2.02	0.42
1:B:335:ASN:HA	1:B:349:ARG:NH1	2.35	0.42
1:F:171:GLU:HA	1:F:201:GLN:HG3	2.01	0.42
1:F:255:LEU:HD23	1:F:255:LEU:HA	1.79	0.42
1:G:20:LEU:HD13	1:G:309:ALA:HA	2.01	0.42
1:G:113:LYS:O	1:G:117:VAL:HG23	2.20	0.42
1:B:248:SER:OG	2:D:75:ARG:NE	2.52	0.41
1:C:620:ALA:O	1:C:624:GLU:HB2	2.20	0.41
1:B:691:THR:O	1:B:695:ILE:HG13	2.20	0.41
2:D:120:ASN:O	2:D:124:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:285:ILE:O	1:G:288:THR:OG1	2.32	0.41
1:G:598:PHE:O	1:G:633:ARG:NH1	2.48	0.41
1:B:234:THR:HG21	2:D:136:LYS:HE3	2.03	0.41
1:B:299:GLY:C	1:B:301:VAL:H	2.28	0.41
1:B:524:ASP:OD1	1:B:524:ASP:N	2.52	0.41
1:C:686:LEU:CD1	1:C:719:VAL:HG21	2.49	0.41
1:F:351:LEU:HD23	1:F:351:LEU:HA	1.89	0.41
1:G:18:ASP:OD2	1:G:345:ARG:NH1	2.53	0.41
1:B:142:GLN:NE2	1:B:220:TYR:OH	2.53	0.41
1:B:181:PRO:O	1:B:185:LEU:N	2.43	0.41
1:B:450:PRO:HA	1:B:451:PRO:HD3	1.94	0.41
1:C:317:VAL:HA	1:C:320:GLU:OE1	2.20	0.41
1:F:194:GLY:HA2	1:F:412:ILE:HG12	2.03	0.41
1:F:227:TYR:HB3	1:F:232:VAL:HG12	2.02	0.41
1:G:227:TYR:H	1:G:233:PHE:HE1	1.67	0.41
2:H:101:GLN:O	2:H:105:LEU:HD12	2.21	0.41
1:B:42:VAL:HB	1:B:81:MET:HE2	2.02	0.41
1:B:337:GLN:OE1	1:C:720:ARG:NH1	2.53	0.41
1:C:663:GLY:O	1:C:692:TYR:OH	2.37	0.41
1:C:668:HIS:HE1	1:C:672:LEU:HB2	1.85	0.41
1:F:37:ASP:OD2	1:F:276:SER:OG	2.35	0.41
1:F:213:GLY:O	1:F:497:ARG:NH2	2.54	0.41
1:F:576:ARG:HB3	1:F:748:HIS:HB2	2.03	0.41
1:G:95:ILE:O	1:G:526:GLN:HG3	2.20	0.41
1:G:668:HIS:NE2	1:G:676:SER:O	2.53	0.41
1:B:476:GLY:O	1:B:480:ARG:HG3	2.20	0.41
1:B:644:ALA:HB1	1:B:668:HIS:HB2	2.03	0.41
2:I:52:GLN:HG3	2:I:56:TYR:CZ	2.55	0.41
1:B:155:ILE:HG13	1:B:183:ASN:HD22	1.86	0.41
2:H:48:ARG:HH12	2:H:80:ILE:HG23	1.85	0.41
1:C:328:ASP:OD2	2:E:66:ARG:NE	2.54	0.41
1:F:366:SER:HB2	1:F:378:SER:CB	2.45	0.41
1:F:420:ILE:HD12	1:F:420:ILE:HA	1.87	0.41
3:F:2601:B12:H602	3:F:2601:B12:H542	1.07	0.41
1:G:201:GLN:OE1	1:G:222:GLU:HB3	2.20	0.41
1:B:214:MET:HE2	1:B:253:ARG:NE	2.36	0.41
2:D:58:ALA:HB2	2:D:73:PHE:HB2	2.02	0.41
1:F:106:THR:OG1	1:F:326:MET:O	2.34	0.41
1:F:344:ILE:HD12	1:G:387:ASP:OD2	2.21	0.41
1:F:669:GLN:OE1	1:F:671:ASP:N	2.52	0.41
1:F:698:ASN:HD22	1:F:708:PRO:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2601:B12:C5	3:F:2601:B12:H4B	2.51	0.41
1:G:204:VAL:CG1	1:G:205:GLU:H	2.28	0.41
1:G:625:GLU:O	1:G:704:ARG:NH1	2.54	0.41
1:B:340:SER:OG	1:B:345:ARG:HD3	2.21	0.41
1:B:586:ARG:NH2	1:B:588:ASP:OD2	2.54	0.41
1:B:583:ALA:HB2	1:B:650:LEU:HD23	2.02	0.40
1:C:365:TYR:CE2	1:C:380:PHE:HB3	2.56	0.40
1:G:230:GLU:OE2	2:I:134:ARG:NE	2.53	0.40
1:G:548:VAL:HG23	1:G:548:VAL:O	2.21	0.40
1:B:215:ARG:NH1	1:B:468:ASN:HA	2.36	0.40
1:C:491:LEU:O	1:C:495:ARG:HG3	2.20	0.40
3:C:2601:B12:H541	3:C:2601:B12:H602	1.69	0.40
2:D:97:PHE:CE1	2:D:136:LYS:HA	2.57	0.40
1:F:519:VAL:HG22	2:H:64:MET:HG3	2.03	0.40
1:G:122:ASN:O	1:G:126:MET:HG3	2.21	0.40
1:C:597:ALA:HB3	1:C:734:GLU:HG3	2.04	0.40
3:C:2601:B12:H253	3:C:2601:B12:H301	1.68	0.40
1:F:294:GLN:HB2	1:F:505:THR:HA	2.03	0.40
1:G:143:CYS:HB3	1:G:167:PHE:CG	2.56	0.40
1:G:317:VAL:HA	1:G:320:GLU:OE1	2.21	0.40
1:B:66:PHE:HB2	1:B:241:TRP:CZ3	2.56	0.40
1:C:644:ALA:HB1	1:C:668:HIS:HB2	2.01	0.40
1:F:181:PRO:HG2	1:F:461:VAL:CG2	2.52	0.40
1:B:112:ALA:HA	1:B:115:VAL:HG22	2.03	0.40
1:B:409:THR:HG21	1:C:7:PHE:HE1	1.85	0.40
2:D:95:ARG:HB3	2:D:96:PRO:HD2	2.02	0.40
2:E:86:ARG:HH21	2:E:110:GLU:CD	2.30	0.40
1:F:45:ASP:HB3	1:F:50:VAL:HG11	2.02	0.40
1:F:324:ALA:O	1:F:329:LEU:HB2	2.22	0.40
1:G:679:GLU:OE2	1:G:710:PRO:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	740/754 (98%)	704 (95%)	32 (4%)	4 (0%)	24	56
1	C	742/754 (98%)	705 (95%)	34 (5%)	3 (0%)	30	60
1	F	732/754 (97%)	697 (95%)	33 (4%)	2 (0%)	36	65
1	G	743/754 (98%)	699 (94%)	40 (5%)	4 (0%)	24	56
2	D	135/141 (96%)	132 (98%)	3 (2%)	0	100	100
2	E	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
2	H	138/141 (98%)	131 (95%)	7 (5%)	0	100	100
2	I	139/141 (99%)	135 (97%)	3 (2%)	1 (1%)	18	50
All	All	3506/3580 (98%)	3335 (95%)	157 (4%)	14 (0%)	30	60

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	364	GLY
1	C	301	VAL
1	C	364	GLY
1	C	569	PRO
1	F	364	GLY
1	G	364	GLY
1	G	566	GLN
1	B	301	VAL
1	B	600	LYS
1	F	301	VAL
1	G	301	VAL
1	B	261	SER
1	G	568	GLN
2	I	47	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	607/619 (98%)	607 (100%)	0	100	100
1	C	611/619 (99%)	611 (100%)	0	100	100
1	F	600/619 (97%)	600 (100%)	0	100	100
1	G	611/619 (99%)	611 (100%)	0	100	100
2	D	116/120 (97%)	116 (100%)	0	100	100
2	E	118/120 (98%)	118 (100%)	0	100	100
2	H	118/120 (98%)	118 (100%)	0	100	100
2	I	118/120 (98%)	118 (100%)	0	100	100
All	All	2899/2956 (98%)	2899 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	ASN
1	B	131	GLN
1	B	142	GLN
1	B	151	ASN
1	B	492	ASN
1	B	737	HIS
1	C	73	ASN
1	C	141	ASN
1	C	201	GLN
1	C	321	ASN
1	C	544	ASN
1	C	731	HIS
2	D	92	ASN
2	D	120	ASN
2	E	65	GLN
2	E	67	HIS
2	E	72	ASN
2	E	132	GLN
1	F	142	GLN
1	F	201	GLN
1	F	321	ASN
1	F	353	GLN
1	F	414	GLN
1	F	496	GLN
1	F	602	GLN

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Mol	Chain	Res	Type
1	F	660	GLN
1	G	16	ASN
1	G	73	ASN
1	G	183	ASN
1	G	201	GLN
1	G	294	GLN
1	G	321	ASN
1	G	335	ASN
1	G	341	HIS
1	G	353	GLN
1	G	414	GLN
1	G	550	GLN
1	G	568	GLN
1	G	601	HIS
1	G	628	HIS
1	G	737	HIS
1	G	748	HIS
2	H	57	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	B12	B	2601	-	93,101,101	1.32	12 (12%)	146,166,166	2.33	44 (30%)
3	B12	C	2601	-	93,101,101	1.37	12 (12%)	146,166,166	2.27	33 (22%)
3	B12	F	2601	-	93,101,101	1.41	13 (13%)	146,166,166	2.97	48 (32%)
3	B12	F	2602	-	93,101,101	1.34	15 (16%)	146,166,166	2.28	37 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B12	B	2601	-	-	20/56/223/223	0/3/11/11
3	B12	C	2601	-	-	32/56/223/223	0/3/11/11
3	B12	F	2601	-	-	19/56/223/223	0/3/11/11
3	B12	F	2602	-	-	14/56/223/223	0/3/11/11

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2601	B12	C14-N23	-6.29	1.27	1.35
3	B	2601	B12	C8B-C9B	5.15	1.49	1.40
3	F	2602	B12	C9-N22	4.95	1.43	1.30
3	C	2601	B12	C8B-C9B	4.74	1.48	1.40
3	F	2601	B12	C8B-C9B	4.59	1.48	1.40
3	B	2601	B12	C9-N22	4.40	1.42	1.30
3	F	2602	B12	C8B-C9B	4.17	1.47	1.40
3	F	2601	B12	C16-C15	-3.90	1.33	1.44
3	F	2601	B12	C18-C19	-3.67	1.45	1.53
3	F	2601	B12	C60-C18	-3.59	1.45	1.54
3	B	2601	B12	C9B-N3B	-3.50	1.33	1.39
3	F	2601	B12	C9B-N3B	-3.38	1.33	1.39
3	C	2601	B12	C6B-C5B	3.35	1.49	1.40
3	B	2601	B12	C14-N23	-3.34	1.30	1.35
3	F	2602	B12	C8B-N1B	-3.32	1.32	1.39
3	F	2601	B12	C12-C11	-3.19	1.46	1.52
3	F	2602	B12	C9B-N3B	-3.12	1.34	1.39
3	C	2601	B12	C8B-N1B	-3.10	1.33	1.39
3	B	2601	B12	C6B-C5B	3.05	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2601	B12	C16-C15	-3.04	1.36	1.44
3	C	2601	B12	C9B-N3B	-3.01	1.34	1.39
3	F	2601	B12	C6B-C5B	2.99	1.48	1.40
3	B	2601	B12	C10-C9	2.93	1.47	1.39
3	F	2601	B12	C9-N22	2.91	1.38	1.30
3	C	2601	B12	C9-N22	2.91	1.38	1.30
3	F	2601	B12	C1-C2	-2.87	1.52	1.58
3	F	2601	B12	C8B-N1B	-2.78	1.33	1.39
3	F	2602	B12	C1-C2	-2.75	1.52	1.58
3	F	2602	B12	C19-N24	2.67	1.53	1.48
3	F	2602	B12	C18-C19	-2.67	1.48	1.53
3	C	2601	B12	C11-N23	2.60	1.42	1.37
3	C	2601	B12	C1-C2	-2.59	1.52	1.58
3	B	2601	B12	C14-C15	2.58	1.49	1.38
3	F	2602	B12	C11-N23	2.56	1.42	1.37
3	F	2602	B12	C20-C1	-2.48	1.48	1.53
3	C	2601	B12	C16-C15	-2.43	1.37	1.44
3	F	2601	B12	C14-C15	2.37	1.48	1.38
3	C	2601	B12	C14-C15	2.34	1.48	1.38
3	B	2601	B12	C18-C19	-2.34	1.48	1.53
3	F	2602	B12	C10-C11	-2.32	1.30	1.38
3	B	2601	B12	C8B-N1B	-2.30	1.34	1.39
3	F	2601	B12	C60-C61	-2.24	1.45	1.51
3	F	2602	B12	C6B-C5B	2.17	1.46	1.40
3	C	2601	B12	C10-C9	2.14	1.45	1.39
3	C	2601	B12	C2B-N1B	-2.13	1.33	1.37
3	F	2602	B12	C10-C9	2.12	1.45	1.39
3	F	2602	B12	C14-N23	2.12	1.37	1.35
3	F	2601	B12	C10-C9	2.11	1.45	1.39
3	F	2602	B12	C12-C11	-2.07	1.48	1.52
3	F	2602	B12	C2B-N3B	2.05	1.35	1.31
3	B	2601	B12	C1-C2	-2.05	1.54	1.58
3	B	2601	B12	C7-C6	-2.03	1.49	1.54

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2601	B12	C20-C1-C19	-12.98	96.85	109.36
3	C	2601	B12	C20-C1-C19	-12.21	97.59	109.36
3	F	2602	B12	C1-C19-C18	10.70	139.44	121.88
3	B	2601	B12	C1-C19-N24	10.24	117.76	106.24
3	B	2601	B12	C20-C1-C19	-9.57	100.13	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2601	B12	C60-C18-C19	-9.40	90.11	114.62
3	F	2601	B12	C1-C19-C18	8.78	136.30	121.88
3	F	2601	B12	C9-C10-C11	-8.76	113.30	125.97
3	F	2602	B12	C19-C1-N21	7.93	110.29	102.16
3	F	2601	B12	C18-C60-C61	-7.67	94.83	113.97
3	F	2601	B12	C17-C16-C15	7.50	138.06	126.26
3	F	2601	B12	C13-C12-C11	-7.42	92.57	100.97
3	B	2601	B12	C2-C1-C19	7.36	130.22	118.60
3	F	2601	B12	C1-C19-N24	7.30	114.46	106.24
3	C	2601	B12	C19-C1-N21	7.21	109.55	102.16
3	C	2601	B12	C18-C19-N24	6.86	112.76	102.31
3	F	2601	B12	C19-C1-N21	6.48	108.80	102.16
3	C	2601	B12	C20-C1-C2	-6.43	102.55	113.28
3	F	2601	B12	C48-C13-C12	-6.36	98.82	116.63
3	B	2601	B12	C18-C60-C61	-6.32	98.19	113.97
3	C	2601	B12	C1-C19-N24	6.04	113.04	106.24
3	C	2601	B12	C2-C1-C19	5.97	128.02	118.60
3	F	2602	B12	C48-C13-C12	-5.85	100.23	116.63
3	F	2602	B12	C18-C17-C16	5.78	107.69	100.67
3	F	2602	B12	C54-C17-C18	-5.71	104.56	112.98
3	B	2601	B12	C18-C19-N24	5.70	110.98	102.31
3	F	2601	B12	C36-C7-C8	-5.68	101.57	112.08
3	F	2602	B12	C20-C1-C19	-5.56	104.00	109.36
3	F	2601	B12	C54-C17-C18	-5.51	104.85	112.98
3	F	2602	B12	C18-C19-N24	5.42	110.56	102.31
3	F	2601	B12	C60-C61-N62	-5.35	103.33	116.21
3	F	2601	B12	C2-C1-C19	5.25	126.88	118.60
3	F	2601	B12	C60-C18-C17	-5.16	103.24	115.74
3	F	2601	B12	C17-C16-N24	-5.06	103.36	111.15
3	F	2601	B12	C30-C3-C4	4.94	121.12	109.63
3	B	2601	B12	C12-C11-N23	-4.87	105.04	111.83
3	F	2601	B12	C17-C18-C19	4.84	109.76	102.36
3	F	2602	B12	C48-C13-C14	4.83	120.52	108.49
3	C	2601	B12	C54-C17-C18	-4.83	105.86	112.98
3	B	2601	B12	C48-C13-C14	4.76	120.35	108.49
3	F	2602	B12	C55-C56-C57	-4.69	100.98	111.23
3	F	2602	B12	C2-C1-C19	4.61	125.88	118.60
3	F	2601	B12	C18-C17-C16	4.50	106.13	100.67
3	B	2601	B12	C26-C2-C1	4.49	117.00	110.01
3	B	2601	B12	C9-C10-C11	-4.45	119.53	125.97
3	C	2601	B12	C18-C17-C16	4.40	106.02	100.67
3	F	2602	B12	C36-C7-C8	-4.39	103.97	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2601	B12	C15-C16-N24	-4.37	116.13	122.42
3	F	2602	B12	C5-C4-N21	-4.36	117.12	124.19
3	F	2602	B12	C20-C1-C2	-4.20	106.27	113.28
3	F	2601	B12	C30-C3-C2	-4.17	110.27	119.09
3	C	2601	B12	C9B-C8B-N1B	4.08	107.07	105.35
3	C	2601	B12	C8B-C9B-N3B	-4.05	105.49	109.97
3	B	2601	B12	C18-C17-C16	4.01	105.54	100.67
3	F	2601	B12	C10-C11-N23	4.00	131.26	124.43
3	B	2601	B12	C54-C17-C18	-3.99	107.09	112.98
3	C	2601	B12	C18-C60-C61	-3.96	104.09	113.97
3	C	2601	B12	C13-C12-C11	-3.92	96.53	100.97
3	B	2601	B12	C17-C16-C15	3.92	132.43	126.26
3	F	2601	B12	C7-C8-C9	3.86	105.85	100.90
3	B	2601	B12	C36-C7-C37	3.80	117.07	110.80
3	C	2601	B12	C1-C19-C18	3.78	128.09	121.88
3	F	2602	B12	C26-C2-C3	3.76	114.06	107.41
3	C	2601	B12	C53-C15-C14	-3.74	110.89	118.43
3	C	2601	B12	C56-C55-C17	-3.74	108.31	115.52
3	F	2602	B12	C18-C60-C61	-3.72	104.70	113.97
3	C	2601	B12	C17-C16-C15	3.66	132.03	126.26
3	C	2601	B12	C9-C10-C11	-3.56	120.82	125.97
3	F	2601	B12	C12-C11-C10	-3.55	118.75	123.37
3	B	2601	B12	C8B-C9B-N3B	-3.53	106.08	109.97
3	F	2601	B12	C8B-C9B-N3B	-3.49	106.12	109.97
3	F	2601	B12	C1P-N59-C57	-3.39	115.31	122.69
3	F	2602	B12	C3-C4-C5	3.37	129.48	123.81
3	F	2602	B12	C30-C3-C4	3.33	117.38	109.63
3	B	2601	B12	C37-C7-C6	3.29	117.46	107.12
3	F	2602	B12	C8B-C9B-N3B	-3.26	106.37	109.97
3	C	2601	B12	C48-C13-C14	3.25	116.59	108.49
3	F	2602	B12	C41-C8-C7	-3.24	105.21	114.14
3	B	2601	B12	C25-C2-C1	-3.23	108.90	113.78
3	F	2601	B12	C20-C1-N21	3.20	115.52	110.27
3	C	2601	B12	C26-C2-C3	3.13	112.94	107.41
3	B	2601	B12	C41-C8-C7	-3.12	105.54	114.14
3	B	2601	B12	C36-C7-C6	-3.12	96.20	112.40
3	B	2601	B12	C7B-C8B-C9B	-3.12	118.82	122.52
3	C	2601	B12	C25-C2-C1	-3.09	109.13	113.78
3	F	2602	B12	C9B-C8B-N1B	2.96	106.60	105.35
3	F	2601	B12	C20-C1-C2	-2.96	108.34	113.28
3	F	2602	B12	C9-C10-C11	-2.96	121.69	125.97
3	F	2601	B12	C5-C6-N22	-2.94	119.38	123.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2601	B12	C1-C19-C18	2.92	126.67	121.88
3	C	2601	B12	C20-C1-N21	2.90	115.02	110.27
3	F	2602	B12	C6-C5-C4	-2.88	116.38	121.54
3	C	2601	B12	C53-C15-C16	2.88	125.33	120.38
3	F	2601	B12	C10-C9-N22	2.87	129.03	125.73
3	F	2601	B12	C3-C4-N21	-2.85	108.39	111.97
3	F	2601	B12	C13-C14-N23	-2.82	105.26	109.10
3	B	2601	B12	C17-C16-N24	-2.81	106.82	111.15
3	F	2601	B12	O63-C61-N62	2.80	130.14	122.50
3	B	2601	B12	C20-C1-C2	-2.75	108.69	113.28
3	C	2601	B12	C30-C3-C4	2.75	116.04	109.63
3	F	2602	B12	C7-C6-N22	2.75	112.96	107.94
3	F	2601	B12	C9B-N3B-C2B	2.74	107.71	104.44
3	B	2601	B12	C13-C14-C15	-2.74	120.14	124.32
3	F	2602	B12	C6M-C6B-C5B	-2.73	115.15	120.74
3	C	2601	B12	C41-C8-C9	2.72	115.99	111.19
3	F	2602	B12	C2P-C1P-N59	-2.72	108.93	112.93
3	F	2602	B12	C30-C3-C2	-2.71	113.35	119.09
3	B	2601	B12	C13-C12-C11	-2.71	97.90	100.97
3	F	2602	B12	C37-C7-C8	2.71	115.64	108.39
3	F	2601	B12	C26-C2-C3	2.69	112.17	107.41
3	B	2601	B12	C35-C5-C6	2.67	126.69	122.43
3	C	2601	B12	O3-C2P-C1P	2.65	112.20	106.92
3	B	2601	B12	C9B-C8B-N1B	2.64	106.46	105.35
3	C	2601	B12	C10-C11-N23	2.63	128.93	124.43
3	C	2601	B12	C26-C2-C1	2.63	114.11	110.01
3	C	2601	B12	C36-C7-C8	-2.63	107.22	112.08
3	C	2601	B12	C9B-N3B-C2B	2.63	107.57	104.44
3	F	2601	B12	C7B-C8B-C9B	-2.61	119.43	122.52
3	F	2601	B12	O63-C61-C60	2.60	126.35	120.87
3	B	2601	B12	C9B-N3B-C2B	2.60	107.53	104.44
3	B	2601	B12	C48-C13-C12	-2.59	109.38	116.63
3	B	2601	B12	C3-C4-N21	-2.54	108.79	111.97
3	F	2602	B12	C25-C2-C1	-2.53	109.97	113.78
3	B	2601	B12	C20-C1-N21	2.52	114.40	110.27
3	B	2601	B12	C8-C7-C6	2.51	105.24	100.92
3	B	2601	B12	C35-C5-C4	-2.51	111.67	116.79
3	B	2601	B12	C56-C55-C17	-2.51	110.68	115.52
3	F	2601	B12	C25-C2-C1	-2.51	110.00	113.78
3	F	2601	B12	C8-C9-C10	-2.50	117.92	123.32
3	F	2602	B12	C1P-N59-C57	-2.50	117.24	122.69
3	F	2601	B12	C47-C12-C46	2.50	113.57	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2602	B12	C9B-N3B-C2B	2.49	107.41	104.44
3	F	2602	B12	C25-C2-C3	-2.47	106.64	112.96
3	B	2601	B12	C4B-C9B-C8B	2.47	122.52	120.15
3	C	2601	B12	C17-C16-N24	-2.45	107.37	111.15
3	F	2601	B12	C2P-C1P-N59	-2.43	109.36	112.93
3	B	2601	B12	C12-C11-C10	2.40	126.49	123.37
3	B	2601	B12	C41-C42-C43	-2.40	104.46	112.59
3	F	2602	B12	C5M-C5B-C4B	2.37	123.87	119.49
3	F	2601	B12	C48-C49-C50	2.35	120.57	112.59
3	F	2601	B12	C56-C55-C17	-2.35	110.99	115.52
3	F	2602	B12	C20-C1-N21	-2.34	106.42	110.27
3	B	2601	B12	C25-C2-C3	-2.34	106.97	112.96
3	B	2601	B12	C3R-C2R-C1R	2.34	105.08	99.89
3	F	2601	B12	C9B-C8B-N1B	2.31	106.33	105.35
3	B	2601	B12	C1-C2-C3	2.30	104.54	101.60
3	C	2601	B12	C12-C11-N23	-2.30	108.62	111.83
3	F	2601	B12	C41-C42-C43	-2.30	104.80	112.59
3	F	2602	B12	C3R-C2R-C1R	2.27	104.91	99.89
3	F	2602	B12	C15-C16-N24	-2.27	119.16	122.42
3	F	2601	B12	C49-C48-C13	2.26	121.26	114.73
3	B	2601	B12	C12-C13-C14	-2.25	98.49	102.26
3	B	2601	B12	C5-C6-N22	-2.23	120.47	123.88
3	C	2601	B12	C5-C6-N22	-2.21	120.50	123.88
3	B	2601	B12	C30-C3-C2	-2.21	114.41	119.09
3	C	2601	B12	C10-C9-N22	2.14	128.18	125.73
3	B	2601	B12	C55-C17-C18	-2.12	107.05	111.15
3	F	2602	B12	C53-C15-C14	-2.11	114.19	118.43
3	F	2602	B12	C35-C5-C4	2.09	121.06	116.79
3	F	2601	B12	C5-C4-N21	2.09	127.58	124.19
3	F	2601	B12	C12-C11-N23	-2.06	108.96	111.83
3	B	2601	B12	C8B-N1B-C1R	2.00	128.79	125.39

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2601	B12	C2-C3-C30-C31
3	B	2601	B12	C4-C3-C30-C31
3	B	2601	B12	C38-C37-C7-C6
3	B	2601	B12	C38-C37-C7-C36
3	B	2601	B12	C7-C37-C38-O39
3	B	2601	B12	C16-C17-C55-C56

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Mol	Chain	Res	Type	Atoms
3	B	2601	B12	C54-C17-C55-C56
3	B	2601	B12	C18-C17-C55-C56
3	B	2601	B12	C56-C57-N59-C1P
3	B	2601	B12	O58-C57-N59-C1P
3	C	2601	B12	C1-C2-C26-C27
3	C	2601	B12	C25-C2-C26-C27
3	C	2601	B12	C38-C37-C7-C36
3	C	2601	B12	C42-C41-C8-C9
3	C	2601	B12	C16-C17-C55-C56
3	C	2601	B12	C54-C17-C55-C56
3	C	2601	B12	C18-C17-C55-C56
3	C	2601	B12	C56-C57-N59-C1P
3	C	2601	B12	N59-C1P-C2P-C3P
3	C	2601	B12	N59-C1P-C2P-O3
3	C	2601	B12	C2P-O3-P-O2
3	C	2601	B12	C3R-O2-P-O5
3	F	2601	B12	C1-C2-C26-C27
3	F	2601	B12	C25-C2-C26-C27
3	F	2601	B12	C3-C2-C26-C27
3	F	2601	B12	C2-C3-C30-C31
3	F	2601	B12	C4-C3-C30-C31
3	F	2601	B12	C38-C37-C7-C6
3	F	2601	B12	C38-C37-C7-C36
3	F	2601	B12	C38-C37-C7-C8
3	F	2601	B12	C42-C41-C8-C7
3	F	2601	B12	C42-C41-C8-C9
3	F	2601	B12	C12-C13-C48-C49
3	F	2601	B12	C14-C13-C48-C49
3	F	2601	B12	C16-C17-C55-C56
3	F	2601	B12	C54-C17-C55-C56
3	F	2602	B12	C1-C2-C26-C27
3	F	2602	B12	C25-C2-C26-C27
3	F	2602	B12	C3-C2-C26-C27
3	F	2602	B12	C38-C37-C7-C6
3	F	2602	B12	C38-C37-C7-C8
3	F	2602	B12	C8-C41-C42-C43
3	F	2602	B12	C12-C13-C48-C49
3	F	2602	B12	C14-C13-C48-C49
3	C	2601	B12	O58-C57-N59-C1P
3	F	2602	B12	O6R-C4R-C5R-O8R
3	C	2601	B12	C42-C41-C8-C7
3	F	2602	B12	C3R-C4R-C5R-O8R

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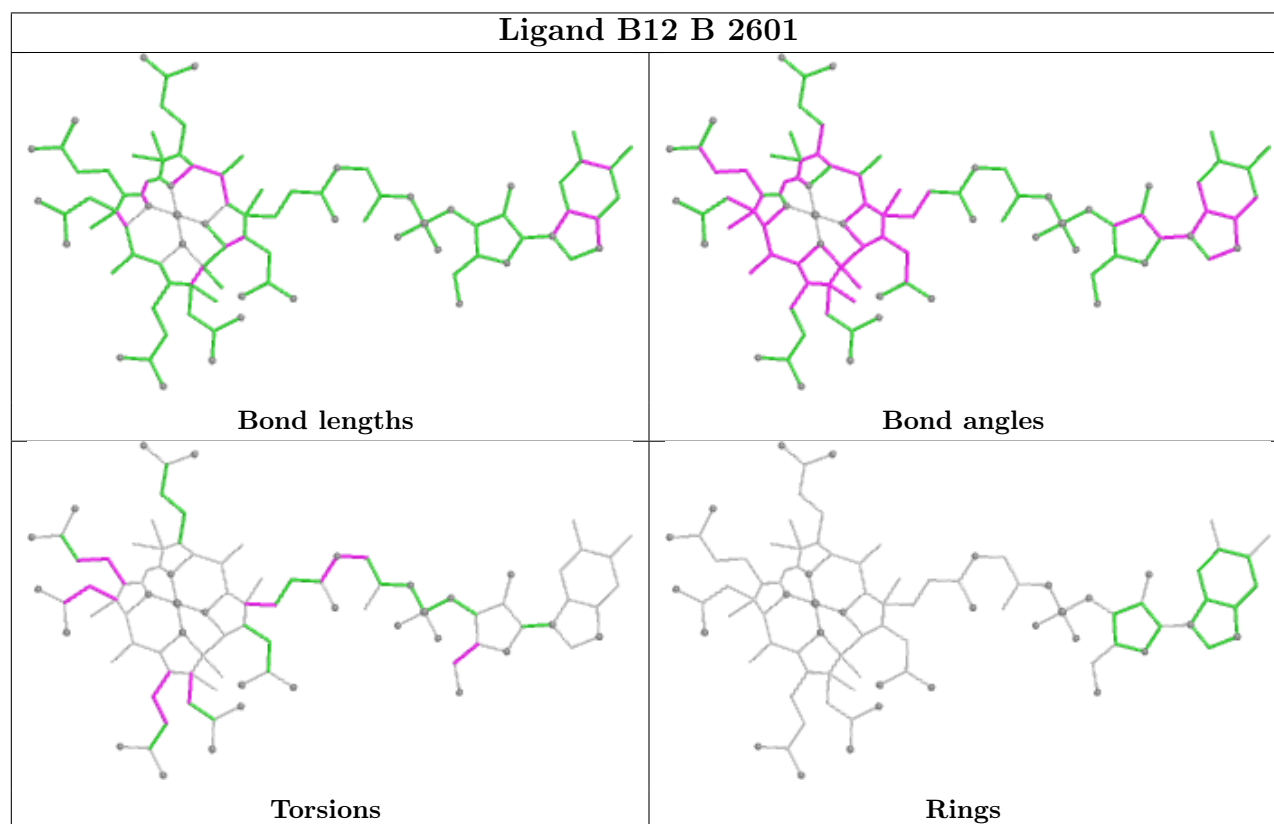
Mol	Chain	Res	Type	Atoms
3	C	2601	B12	C4-C3-C30-C31
3	F	2601	B12	C8-C41-C42-C43
3	F	2602	B12	C13-C48-C49-C50
3	B	2601	B12	O6R-C4R-C5R-O8R
3	C	2601	B12	O6R-C4R-C5R-O8R
3	B	2601	B12	C7-C37-C38-N40
3	F	2601	B12	O6R-C4R-C5R-O8R
3	B	2601	B12	C3R-C4R-C5R-O8R
3	C	2601	B12	C3R-C4R-C5R-O8R
3	C	2601	B12	C12-C13-C48-C49
3	C	2601	B12	C3R-O2-P-O3
3	B	2601	B12	C1-C2-C26-C27
3	C	2601	B12	C3-C2-C26-C27
3	F	2601	B12	C17-C55-C56-C57
3	F	2601	B12	C3R-C4R-C5R-O8R
3	C	2601	B12	C2-C3-C30-C31
3	B	2601	B12	C8-C41-C42-C43
3	B	2601	B12	C38-C37-C7-C8
3	C	2601	B12	C38-C37-C7-C6
3	C	2601	B12	C55-C56-C57-O58
3	C	2601	B12	C3R-O2-P-O4
3	F	2602	B12	C4-C3-C30-C31
3	C	2601	B12	C1P-C2P-O3-P
3	C	2601	B12	C3P-C2P-O3-P
3	B	2601	B12	C25-C2-C26-C27
3	C	2601	B12	C55-C56-C57-N59
3	F	2602	B12	C3-C30-C31-C32
3	C	2601	B12	C18-C60-C61-O63
3	C	2601	B12	C18-C60-C61-N62
3	C	2601	B12	C38-C37-C7-C8
3	C	2601	B12	C17-C18-C60-C61
3	C	2601	B12	C19-C18-C60-C61
3	B	2601	B12	C2P-C1P-N59-C57
3	B	2601	B12	C42-C41-C8-C9
3	F	2601	B12	C3-C30-C31-C32
3	F	2602	B12	C19-C18-C60-C61
3	B	2601	B12	C3-C30-C31-C32

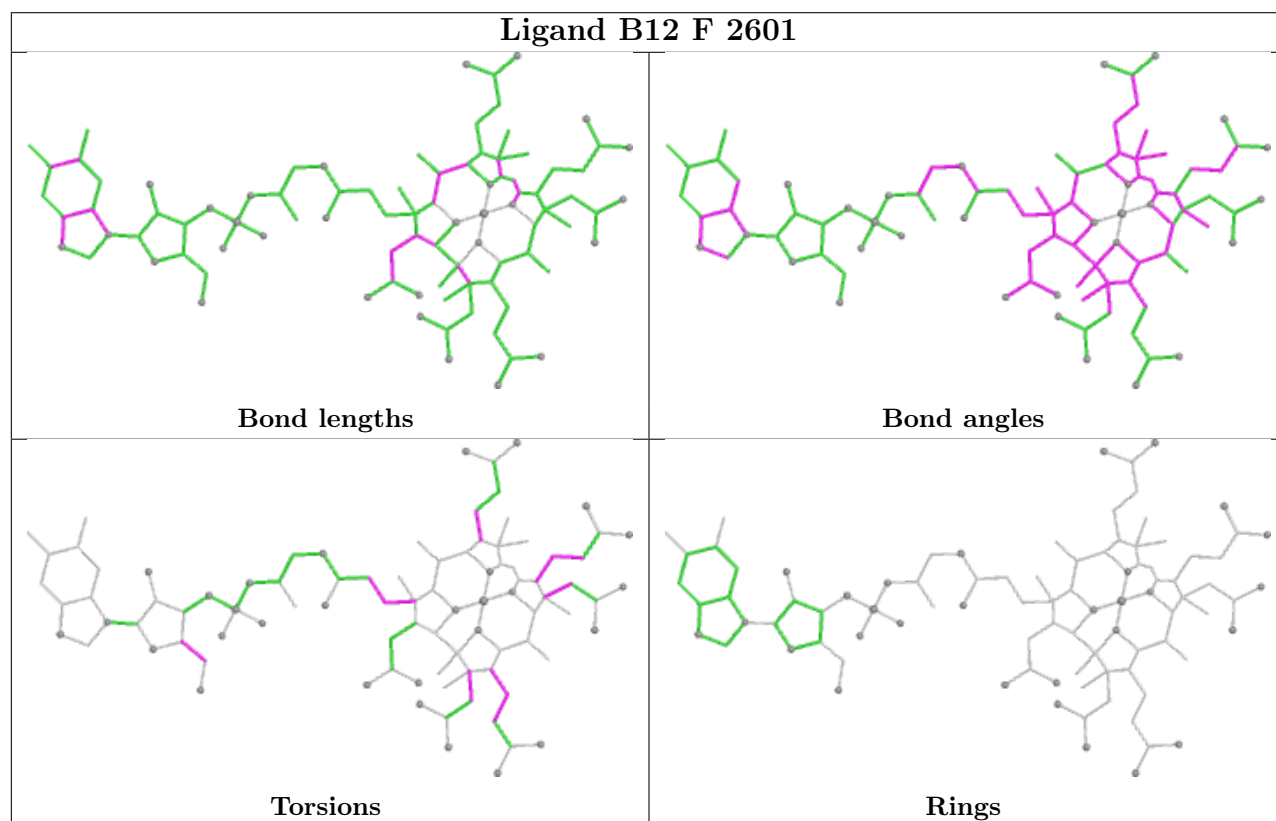
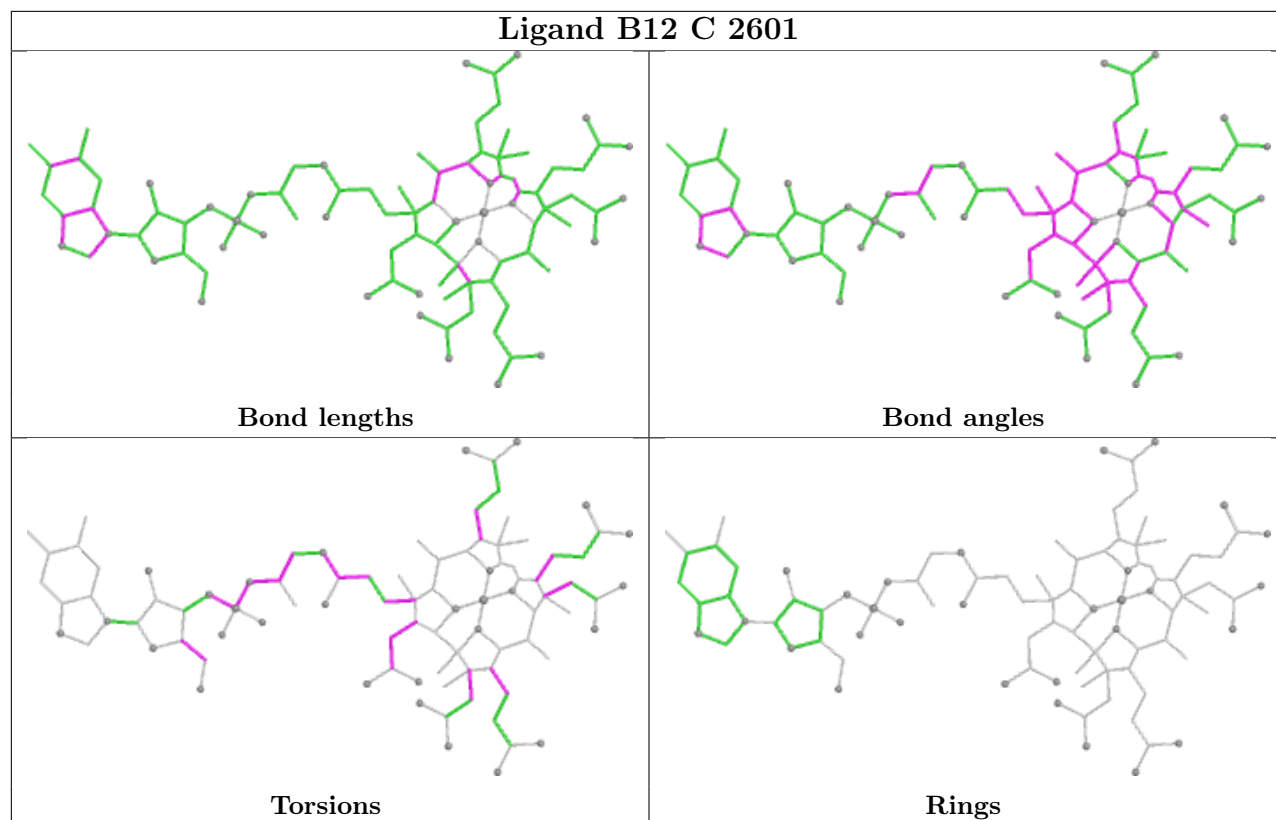
There are no ring outliers.

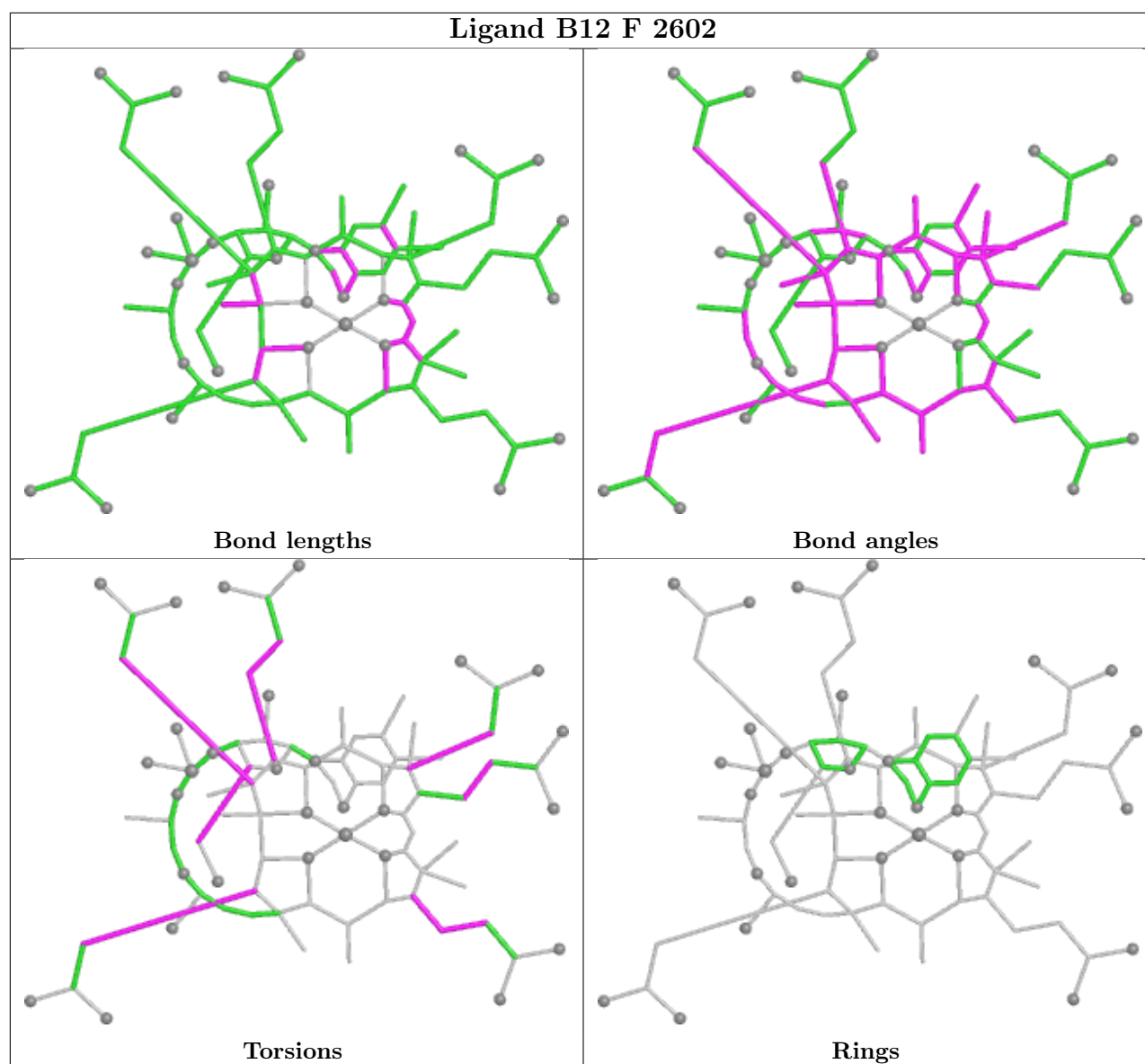
4 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2601	B12	6	0
3	C	2601	B12	8	0
3	F	2601	B12	18	0
3	F	2602	B12	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	744/754 (98%)	-1.57	0 100 100	34, 54, 75, 100	0
1	C	746/754 (98%)	-1.59	0 100 100	32, 50, 69, 106	0
1	F	736/754 (97%)	-1.56	0 100 100	39, 59, 78, 96	0
1	G	747/754 (99%)	-1.57	0 100 100	38, 56, 80, 106	0
2	D	137/141 (97%)	-1.52	0 100 100	53, 70, 88, 96	0
2	E	139/141 (98%)	-1.58	0 100 100	42, 60, 76, 92	0
2	H	140/141 (99%)	-1.52	0 100 100	48, 73, 93, 104	0
2	I	141/141 (100%)	-1.54	0 100 100	56, 72, 87, 108	0
All	All	3530/3580 (98%)	-1.57	0 100 100	32, 56, 82, 108	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

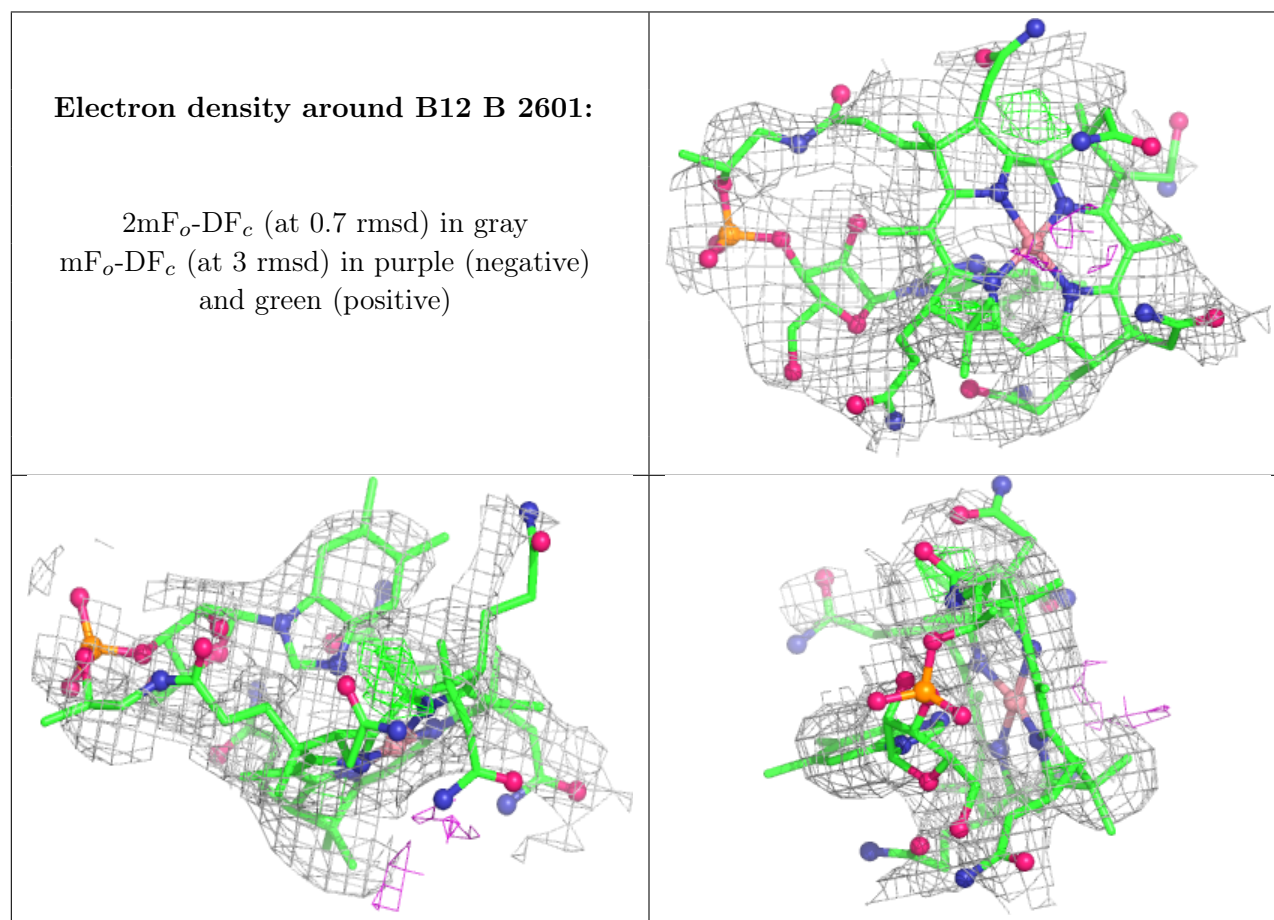
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

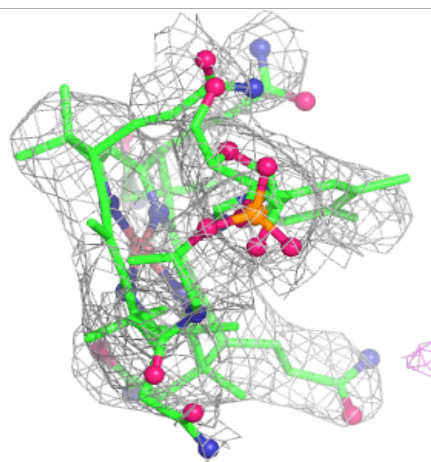
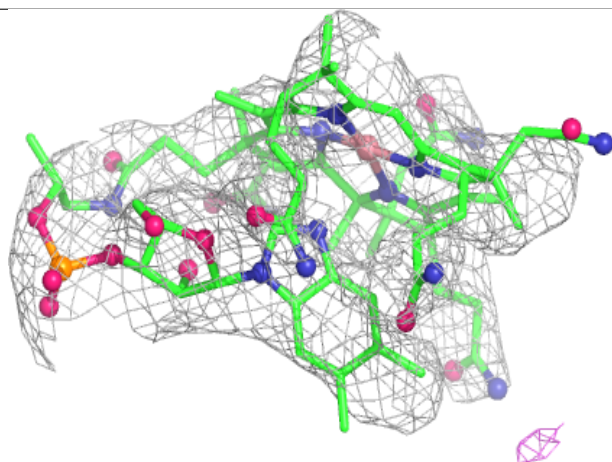
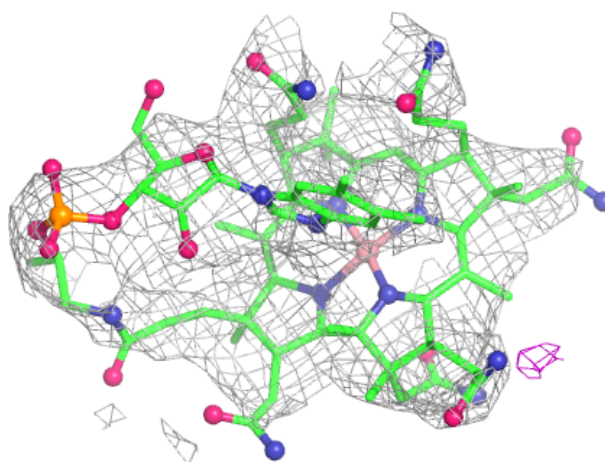
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	B12	B	2601	91/91	1.00	0.04	34,70,84,111	0
3	B12	C	2601	91/91	1.00	0.03	45,72,87,129	0
3	B12	F	2601	91/91	1.00	0.03	41,64,79,86	0
3	B12	F	2602	91/91	1.00	0.03	58,80,90,104	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



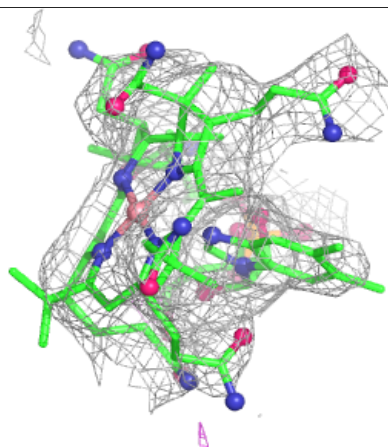
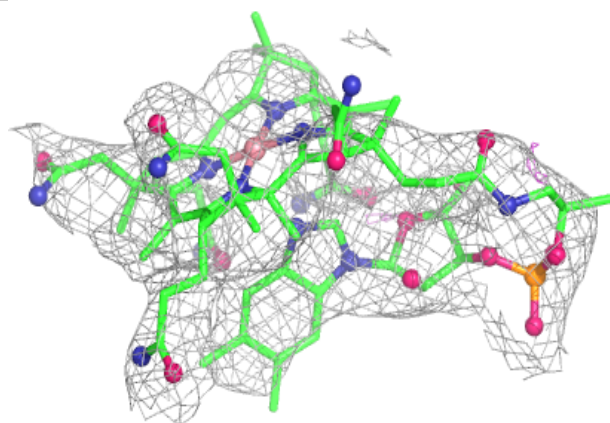
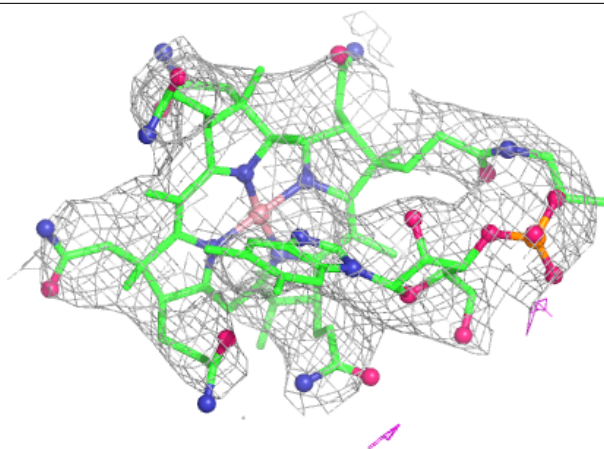
Electron density around B12 C 2601:

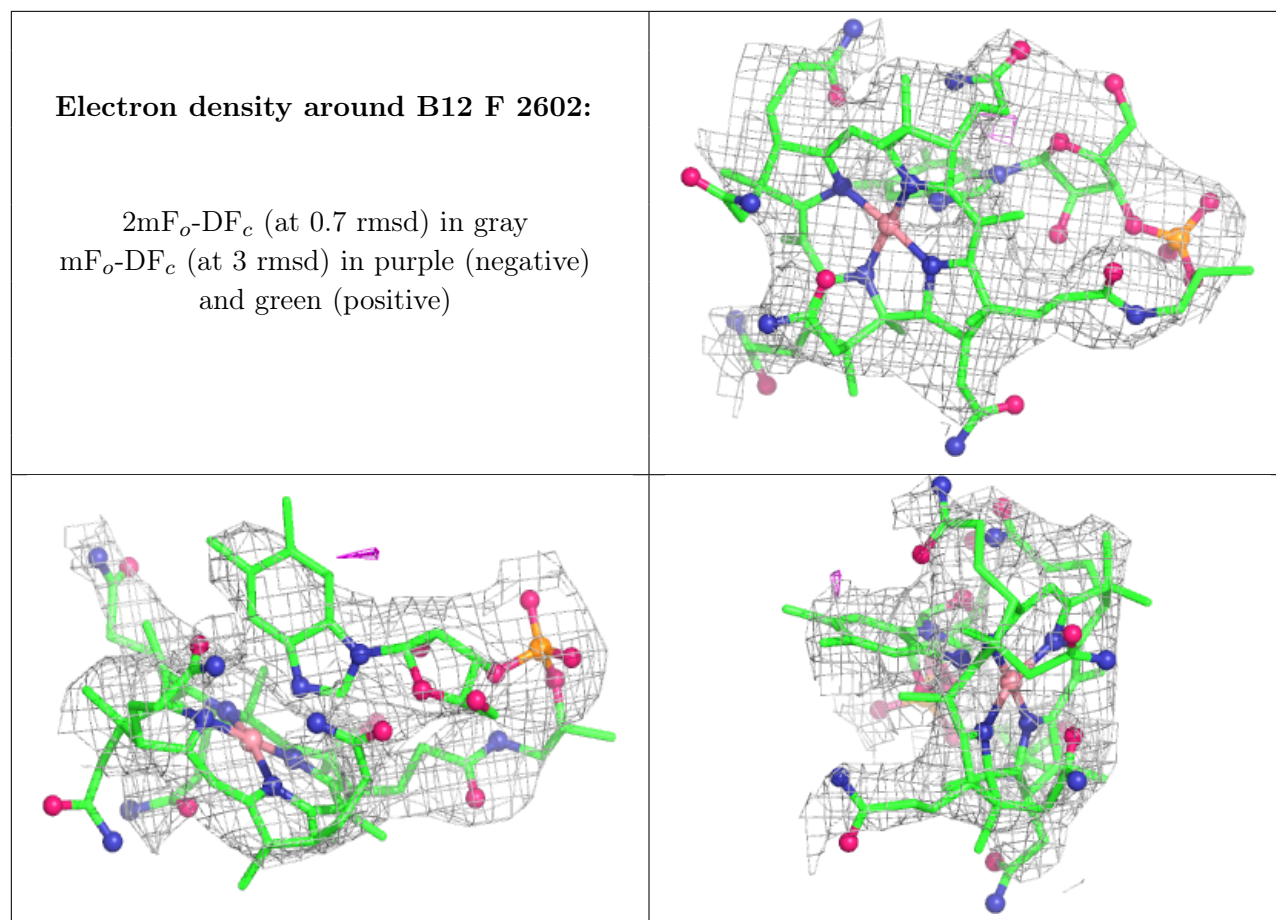
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around B12 F 2601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.